

# SANDIA REPORT

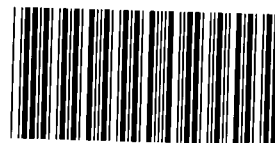
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## Sandia Equation of State Data Base: *seslan* File



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## **Sandia Equation of State Data Base: *seslan* File**

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### **Abstract**

Sandia National Laboratories maintains several libraries of equation of state tables, in a modified Sesame format, for use in hydrocode calculations and other applications. This report discusses one of those libraries, the *seslan* file, which contains 78 tables from the Los Alamos equation of state library. Minor changes have been made to these tables, making them more convenient for code users and reducing numerical difficulties that occasionally arise in hydrocode calculations.

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## 1. Introduction

Sandia National Laboratories (SNL) maintains a data base of tabular equations of state (EOS) for use in hydrodynamics code calculations and other applications. For example, the use of these EOS tables with the three-dimensional Eulerian code CTH [1] is described in Refs. [2] and [3]. This data base uses a modified form of the Sesame format [4] - [7], originally developed at Los Alamos National Laboratory for use in hydrocodes. Special programs, like the Panda code [4], are used to construct the EOS models and generate the tabular data. Detailed information about the Sesame format can be found in Refs. [2] - [7].

When constructing an EOS for a complicated material over a wide range of densities and temperatures, one encounters many theoretical and experimental problems that are still unsolved [8]. Many approaches can be used for this task, each having both strengths and weaknesses. As a result, there is a wide variation in the quality of EOS data available, and it can be quite difficult to assess the suitability of a particular EOS for a specific problem. This difficulty can be reduced, to some degree, by offering users a number of EOS options and by providing documentation about what is available.

Therefore, the Sandia data base maintains several files containing tabular EOS data, along with documentation. The principal files are listed below:

<i>sesame</i>	library of EOS tables recommended and supported by SNL
<i>sesame.ref</i>	ASCII file of on-line information about the data on file <i>sesame</i>
<i>seslan</i>	library of EOS tables from the Los Alamos EOS library
<i>seslan.ref</i>	ASCII file of on-line information about the data on file <i>seslan</i>
<i>aneos</i>	library of EOS tables made using the ANEOS package in CTH
<i>aneos.ref</i>	ASCII file of on-line information about the data on file <i>aneos</i>
<i>jwl</i>	library of tables made using JWL EOS for detonation products
<i>jwl.ref</i>	ASCII file of on-line information about the data on file <i>jwl</i>

The files named *sesame*, *seslan*, *aneos*, and *jwl* contain the EOS tables, in a sequential binary format, that are accessed and downloaded by a hydrocode during execution of a problem. The corresponding *~.ref* files provide documentation that users can consult when deciding which tables to use. All of the above files are available on the SNL Cray and on Unix workstations connected to the 1431 Protected LAN, in the following directories:

Cray/YMP	/usr/community/gkerley
UNIX LAN	/u3/gkerley/libs

This report discusses only two of the files in the SNL database - *seslan* and *seslan.ref* - which consists of 78 EOS tables taken from the Los Alamos library and slightly modified for use in SNL hydrocodes.

## 2. The *seslan* File

### 2.1 General

Seventy-eight materials from the Los Alamos EOS library were chosen to be included on the *seslan* file. Approximately half of them are discussed in Ref. [7]. In addition to the EOS data, the Los Alamos files contain documentation in a Hollerith format. This information is kept separate in the Sandia data base, (*~.ref* files), making it easier for users to access and simpler to maintain on differing computer systems. It was included, along with other comments, in making the *seslan.ref* file, which is listed in the Appendix.

Several criteria were used in selecting the materials to be included. Many of the older EOS tables were passed up, if newer and better versions were available. However, some older versions were included if they offered features that had been omitted in the newer tables - such as Maxwell constructions in the vapor-liquid coexistence region. In addition, there are many materials for which the only existing EOS table is quite old.

Many of the materials chosen are also available on other files in the Sandia data base, giving the user a choice of which EOS to use and the possibility of performing sensitivity studies. Still other materials are presently available only on the *seslan* file, making it the only tabular EOS option in those cases. In either case, a user is advised to consult the documentation in the *~.ref* files and to be aware of limitations of the techniques that were used in making the tables. Some of the potential problems are discussed in Sec. 2.3.

### 2.2 Modifications to the Tables

The following modifications were made to the tables before adding them to file *seslan*. These changes are noted in the *seslan.ref* file, under the heading "MODIFICATIONS."

- A new reference state table (201 table) was constructed for each material, giving the density, temperature, and bulk modulus for an appropriate set of initial conditions (normally zero pressure and room temperature). These data are used for the default initial density and temperature in CTH calculations [2], so that nothing has to be specified by the user except for unusual cases. The default reference states for all materials are listed at the beginning of the *seslan.ref* file.
- To eliminate problems that may be encountered when extrapolating off a table at low densities and/or low temperatures, a zero density isochore and a zero temperature isotherm were added, if they did not already exist.
- For some materials, the tension region at low densities and low temperatures was thermodynamically inconsistent and gave very high sound speeds. In those cases, the pressure table was revised to minimize numerical problems that resulted from this behavior. (See the discussion in the Panda manual [4], pp. 102-104.)

The electron and ion EOS (303 and 304 tables) and the vaporization curve (401 table) have *not* been included in file *seslan*.

## 2.3 Potential Problems

A complete survey of the EOS tables on *seslan*, or any other file in the data base, is beyond the scope of this report. However, the comments on file *seslan.ref* identify any problems or limitations that were noticed during a quick check of each EOS tables. We offer the following comments to make users aware of the kinds of difficulties that may exist in some of the EOS tables in *seslan* and also the other data files.

- The treatment of expanded states (tension and vaporization) creates problems when constructing EOS tables. Ideally, one wishes to allow a tension region at low temperatures, for use with fracture models, while building in a vapor-liquid coexistence region (Maxwell constructions) at high temperatures [4]. Many of the tables available do not have a tension region and so will not predict any spallation; these EOS also give too low a sound speed at the reference state, due to interpolation problems. In other cases, no Maxwell constructions have been created, so that the EOS will not describe vaporization, even at high temperatures.
- In some very old EOS tables, the room-temperature density was used as the zero pressure point on the zero-Kelvin isotherm. As a result, the predicted density at the room temperature reference state is too low in such cases. This problem has been corrected in most of the tables, but there are still some for which no new table has been created.
- A realistic treatment of phase transitions and melting has become possible only recently [8] [9]. Many of the existing tables on the *seslan* file do not treat melting explicitly. Phase transitions, where they occur, are often treated by simple methods.
- Most of the tables employ a very simple treatment of thermal electronic excitation and ionization. Such models will give only a crude prediction of the behavior of shock ionization in gases, for example. With some exceptions (hydrogen and deuterium) many EOS for compounds do not account for the effects of molecular dissociation. Such tables are only valid over a limited range of densities and temperatures.

## References

- [1] J. M. McGlaun, F. J. Ziegler, S. L. Thompson, L. N. Kmetyk, and M. G. Elrick, "CTH - User's Manual and Input Instructions," Sandia National Laboratories report SAND88-0523, April 1988.
- [2] G. I. Kerley, "CTH Reference Manual: The Equation of State Package," Sandia National Laboratories report SAND91-0344, 1991.
- [3] G. I. Kerley, "CTH Equation of State Package: Porosity and Reactive Burn Models," Sandia National Laboratories report SAND92-0553, 1992.
- [4] G. I. Kerley, "User's Manual for PANDA II: A Computer Code for Calculating Equations of State," Sandia National Laboratories report SAND88-2291, 1991.
- [5] B. I. Bennett, J. D. Johnson, G. I. Kerley, and G. T. Rood, "Recent Developments in the Sesame Equation-of-State Library," Los Alamos Scientific Laboratory report LA-7130, 1978.
- [6] N. G. Cooper, "An Invitation to Participate in the LASL Equation of State Library," Los Alamos Scientific Laboratory report LASL-79-62, 1979.
- [7] K. S. Holian, "T-4 Handbook of Material Properties Data Bases," Los Alamos National Laboratory report LA-10160-MS, 1984.
- [8] J. R. Asay and G. I. Kerley, "The Response of Materials to Dynamic Loading," *Int. J. Impact Engng.* **5**, 69-99 (1987).
- [9] G. I. Kerley, "Multiphase Equation of State for Iron," Sandia National Laboratories report SAND93-0027, 1993.



Appendix: File *seslan.ref*

## DOCUMENTATION OF DATA ON SANDIA SESLAN LIBRARY FILE

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05/03/93

The seslan file contains Sesame EOS tables taken from the Los Alamos data base. The 201 table was modified to give a reference state for use in hydro calculations. In some cases, the PANDA code was used to add points at zero density and temperature and to modify the pressure and energy in the tension region.

## 78 Materials on File

Material Name	Material Number	----Reference State Properties----			Table Types
		Density (g/cc)	Temperature (Kelvin)	Sound Speed (km/s)	
Uranium	1540	18.813	290.121	2.423	201. 301.
Beryllium	2020	1.840	290.121	8.051	201. 301.
Beryllium	2022	1.850	290.112	8.050	201. 301.
Iron	2140	7.798	290.121	4.572	201. 301.
Lithium	2291	0.5395	298.000	4.650	201. 301.
Lithium	2293	0.5315	298.152	4.709	201. 301.
Gold	2700	19.151	290.121	2.923	201. 301.
Silver	2720	10.507	298.152	3.046	201. 301.
Ti Alloy	2961	4.447	298.152	4.912	201. 301.
Molybdenum	2980	10.176	290.121	5.013	201. 301.
Nickel	3100	8.824	290.121	4.604	201. 301.
Lead	3200	11.159	290.121	2.048	201. 301.
Copper	3330	8.843	290.121	3.854	201. 301.
Copper	3333	8.930	299.976	3.940	201. 301.
Copper	3336	8.930	299.976	4.015	201. 301.
Tantalum	3520	16.654	298.12	3.434	201. 301.
Tungsten	3541	19.237	298.120	4.023	201. 301.
W alloy	3542	17.346	298.120	4.236	201. 301.
WC	3560	14.970	298.12	4.911	201. 301.
Aluminum	3715	2.700	299.976	5.350	201. 301.
Platinum	3730	21.329	290.121	3.608	201. 301.
Brass	4100	8.329	290.121	3.413	201. 301.
Steel	4270	7.842	290.121	4.529	201. 301.
Nitrogen	5000	0.8572	63.148	0.8626	201. 301.
Oxygen	5010	1.262	54.38	1.036	201. 301.
Dry Air	5030	1.218E-3	298.0	0.3388	201. 301.
Argon	5172	1.407	83.8	0.8638	201. 301.
Krypton	5181	2.490	115.8	0.5722	201. 301.
Xenon	5190	5.391E-3	298.15	0.1770	201. 301.
Hydrogen	5251	8.839E-2	298.15	3.328	201. 301.
Deuterium	5263	0.1766	298.15	2.354	201. 301.
Neon	5410	1.44	290.12	1.094	201. 301.
Methane	5500	0.4263	95.0	0.2429	201. 301.
Helium	5760	0.2339	298.15	1.860	201. 301.
Helium	5761	0.4	298.15	2.903	201. 301.
Dry Sand	7100	2.605	298.152	3.883	201. 301.

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Dry Clay	7102	3.016	298.152	4.312	201. 301.
Nev. Alluvium	7111	1.313	290.121	2.335	201. 301.
Wet Tuff	7120	1.950	298.152	2.415	201. 301.
Wet Tuff	7121	1.950	298.152	2.041	201. 301.
Limestone	7130	2.741	298.152	4.898	201. 301.
Water	7150	1.000	290.121	1.179	201. 301.
PolyCD2	7160	1.048	298.15	2.398	201. 301.
PolyCH2	7171	0.9160	298.15	2.563	201. 301.
PolyCH2	7180	0.9540	298.15	2.8016	201. 301.
Teflon	7190	2.152	298.15	1.591	201. 301.
PolyCD2	7230	1.093	298.15	2.436	201. 301.
Salt	7281	2.165	298.15	3.580	201. 301.
Salt	7282	2.140	298.152	3.332	201. 301.
Salt	7283	2.243	298.152	3.334	201. 301.
Calcite	7330	2.71	290.11	5.211	201. 301.
Calcite	7331	2.712	298.152	5.125	201. 301.
Quartz	7380	2.155	290.121	4.091	201. 301.
Quartz	7381	2.204	293.16	3.87	201. 301.
PolyQuartz	7383	2.650	298.152	3.733	201. 301.
PolyQuartz	7385	2.650	298.152	3.733	201. 301.
Fused Quartz	7386	2.204	298.152	4.137	201. 301.
W. Granite	7390	2.551	290.12	1.970	201. 301.
Alumina	7410	3.961	290.121	7.758	201. 301.
Alumina	7411	3.970	298.15	7.820	201. 301.
Hematite	7440	5.008	298.152	6.215	201. 301.
CaO	7450	2.982	298.152	3.696	201. 301.
MgO	7460	3.585	298.152	6.729	201. 301.
Dolomite	7510	2.823	298.152	5.382	201. 301.
Mica	7520	2.621	290.12	2.193	201. 301.
Basalt	7530	2.866	298.152	5.170	201. 301.
C Phenolic	7541	1.450	298.12	3.052	201. 301.
C Phenolic	7542	1.499	298.152	3.150	201. 301.
Polyurethane	7560	1.013	290.121	2.073	201. 301.
Polyurethane	7561	1.264	298.152	2.073	201. 301.
Polystyrene	7590	0.7623	290.121	0.5538	201. 301.
Polystyrene	7591	0.9918	298.0	0.3166	201. 301.
Polystyrene	7592	1.044	298.152	1.302	201. 301.
Epoxy	7601	1.185	298.152	2.736	201. 301.
Epoxy	7602	1.185	298.129	1.902	201. 301.
BeO	7610	3.01	298.152	8.459	201. 301.
Lucite	7750	1.186	298.152	1.298	201. 301.
Sylgard	7931	1.037	298.15	1.884	201. 301.

## EOS NUMBER 1540

MATERIAL. Uranium (Z=92.0, A=238.03)

SOURCE. J. Barnes, J. Rood

DATE. Mar 73

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. U

CODES. SESAME I, MAPLE, MAXWELL

RANGE. 101 densities, 0., 0.15, 0.28..., 3.8E+5 g/cc,  
23 temperatures, 0., 290.121, ..., 3.7E8 Kelvin.

MODIFICATIONS.

The 201 table was modified to give RREF=18.813, TREF=290.121, and

BREF=110.432 GPa. The value of BREF corresponds to a sound speed of 2.423 km/s.

#### COMMENTS.

- This EOS is quite old - use with caution. One deficiency is that the room temperature density has been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- It has a tension region for temperatures below about 1160 K.
- It is not thermodynamically consistent in the vapor-liquid region, because the Maxwell constructions were put into the pressure table but not into the energy table.
- Only pressure and energy are tabulated in the 301 table. There is no entropy or free energy table.

#### EOS NUMBER 2020

MATERIAL. Beryllium (Z=4.00000, A=9.01200)

SOURCE. J. Barnes, J. Rood

DATE. Mar 73, July 73, Aug 78, Feb 92 (modifications)

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Be

CODES. SESAME I, MAPLE

RANGE. 101 densities, 0., 1.44E-2, 2.75E-2, ..., 3.69E+4 g/cc,  
23 temperatures, 0, 290.12, 580.24, 1160.5, ..., 3.71E8 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give RREF=1.8396, TREF=290.121, and BREF=118.53 GPa. The value of BREF corresponds to a sound speed of 8.051 km/s.
- In the tension region, modifications were made to the 301 table at T<2320K and density<1.59 g/cc to make pressure proportional to density and energy constant.

#### COMMENTS.

- The tension region (for spall) was first added on 8-24-78 by Jerry Rood at the request of Mel Thieme (x-4). The tension region exists for temperatures less than 2320K and for temperatures approximately between 4500 and 5700K.
- This EOS is quite old - use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- Interpolation on the tables produces spurious cross-overs in the pressure isotherms for temperatures greater than ~2100K.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

#### EOS NUMBER 2022

MATERIAL. Beryllium (Z=4, A=9.012)

SOURCE. J. Nash (LLNL), K. Trainor

DATE. June 84 (orig data); Feb 92 (modifications)

REFS. None

COMPOSITION. Be

CODES. Thomas-Fermi plus nuclear corrections, ACTEX (LLNL),  
OCCIPITAL (LLNL), SOFT SPHERE (LANL)

RANGE. 73 densities, 0., 1.0E-4, 1.25E-4, ..., 1000 g/cc,  
43 temperatures, 0., 290.112, 366.7, 464.2, ..., 1.16E8 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give RREF=1.8500, TREF=290.112, BREF=118.5 GPa. The value of BREF corresponds to a sound speed of about 8.05 km/s.
- A  $\rho=0.0$  isochore and T=0.0 isotherm were added to the 301 table.

COMMENTS.

- A global equation of state which covers a wide range of densities and temperatures. The theoretical models which were used to generate the EOS are (1) a soft sphere liquid metal model at temperatures below 1 ev and at densities below the liquid density; (2) a ionization equilibrium model based on a modified saha method in expansion at temperatures between 1 and 5 ev; (3) nonideal plasma theory based on a perturbation expansion of the grand canonical partition function for the higher temperatures in expansion (this is also the ionization equilibrium regime); (4) Thomas-Fermi electronic model with Gruneisen nuclear corrections for the compression EOS.
- A problem with this EOS is that for all practical purposes it does not have a tension region ( $T < 300$  K have a negative value for pressure of  $\sim -E-4$ ), so it will not predict fracture in dynamic calculations. In addition, the interpolation scheme does not give the correct sound speed at ambient density and temperature.
- Pressure, energy and free energy are tabulated in the 301 table.

EOS NUMBER 2140

MATERIAL. Iron ( $Z=26.0$ ,  $A=55.850$ )

SOURCE. J. Barnes, J. Rood

DATE. Aug 73

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"

Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Fe

CODES. SESAME I, MAPLE, MAXWELL

RANGE. 101 densities,  $0., 6.1E-2, \dots, 1.6E+5$  g/cc,

23 temperatures,  $0., 290.121, \dots, 3.7E8$  Kelvin.

MODIFICATIONS.

The 201 table was modified to give RREF=7.798, TREF=290.121, and BREF=163.032 GPa. The value of BREF corresponds to a sound speed of 4.572 km/s.

COMMENTS.

- This EOS is quite old - use with caution. One deficiency is that the room temperature density has been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- One merit of this EOS is that it does include a treatment of the phase transition.
- It has a tension region for temperatures below about 1160 K.
- It is not thermodynamically consistent in the vapor-liquid region, because the Maxwell constructions were put into the pressure table but not into the energy table.
- Only pressure and energy are tabulated in the 301 table. There is no entropy or free energy table.

EOS NUMBER 2291

MATERIAL. Lithium ( $Z=3$ ,  $A=6.939$ )

SOURCE. David A. Young (H-Division, LLNL)

DATE. Feb 83 (orig data); Feb 92 (modifications)

REFS. David A. Young, M. Ross and F. J. Rogers, "A Tabular Equation

of State of Lithium for Laser-Fusion Reactor Studies", LLNL Report UCRL-82182 (January, 1979).

#### COMPOSITION. Li

CODES. Actex, Soft Sphere Liquid Metal Model, Pseudopotential

RANGE. 46 densities, 0., 1.0E-4, 1.25E-4, ..., 2.0 g/cc,

62 temperatures, 0., 453.736, 464.18, 580.22, ..., 3.67E8 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give RREF=0.53947, TREF=298., and BREF=11.5 GPa. The value of BREF corresponds to a sound speed of about 4.65 km/s.
- A rho=0.0 isochore and T=0.0 isotherm were added to the 301 table.

#### COMMENTS.

- Caution - if this EOS is used at temperatures below 454K, use the two-state model to correct the low-temperature region. The 201 table gives a reasonable but approximate reference state.
- This equation of state ranges from 0.039 ev to 31.6 kev and from e-4 to 2.0 gm per cc. It was designed for use in laser fusion reactor simulations, and is not suitable for computations which are expected to reach densities greater than 4-fold compressed. The models used in this eos were 1) a soft sphere liquid metal model at low temperatures ( $t < 0.6$  ev) below rho zero, 2) non-ideal plasma theory (actex) at high temperatures, and 3) a liquid metal perturbation theory based on pseudopotentials for the hot, partially-ionized liquid. Agreement of the theoretical eos with experimental isobaric data (measuring volume, enthalpy and soundspeed) and experimental Hugoniot data is good.
- No zero pressure point exists in this table.
- A problem with this EOS is that it does not have a tension region, so it will not predict fracture in dynamic calculations. In addition, the interpolation scheme does not give correct sound speed at reference temperature and density.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

#### EOS NUMBER 2293

MATERIAL. Lithium (Z=3.00000, A=6.941)

SOURCE. J. Boettger

DATE. Jun 88, Feb 92 (modifications)

REFS. LA-11338-MS

COMPOSITION. Li

CODES. Grizzly, SCLMT7B

RANGE. 70 densities, 0., 5.33E-7, 1.066E-6, ..., 1.066E+4 g/cc,

38 temperatures, 0, 145.1, 298.15, 580.2, ..., 1.16E9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give RREF=0.53149, TREF=298.152, and BREF=11.471 GPa. The value of BREF corresponds to a sound speed of 4.709 km/s.

#### COMMENTS.

- The electronic and nuclear tables are essentially the same as for 2292. The cold curve combines adjusted lnto band structure results for rho greater than or equal to 0.9 rho0 with a Lennard-Jones tail (fac1j=4.0, ecoh=0.231 mbar-cm3). This eos is generally comparable to 2292 but includes a significant shell structure effect in the cold curve for compressions ranging from 2 to 100.
- This EOS does not have Maxwell constructions. There is a tension

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region for temperatures less than 3190K.

- Negative internal energy exists for temperatures less than TREFF.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 2700

MATERIAL. Gold (Z=79.0, A=196.967)

SOURCE. A. Lindstrom, J. Rood

DATE. Jan 76, Aug 78, Feb 92

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984, LBL-3720,  
UCRL-50108

COMPOSITION. Au

CODES. SESAME I, MAPLE, MAXWELL

RANGE. 101 densities, 0., 0.151, .288, ..., 3.86E+5 g/cc,  
23 temperatures, 0, 290.12, 580.2, ..., 3.71E8 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give RREF=19.151, TREF=290.12, and BREF=160.46 GPa. The 301 table predicts a sound speed of 2.923 km/s.
- In the tension region modifications were made to the 301 table at  $T < 2320\text{K}$  and  $\text{density} < 16.767\text{ g/cc}$  to make pressure proportional to density and energy constant.

#### COMMENTS.

- The tension region (for spall) was first added on 8-24-78 by Jerry Rood at the request of Mel Thieme (x-4). The tension region exists for temperatures below 2320K.
- A deficiency of this EOS is that the room temperature density has been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- Interpolation on the tables produces spurious cross-overs in the pressure isotherms for temperatures greater than 3350K.
- This EOS is not thermodynamically consistent in the vapor-liquid region. Maxwell constructions were put into the pressure table but not in the energy table.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

### EOS NUMBER 2720

MATERIAL. Silver (Z=47, A=107.868)

SOURCE. J. Johnson, S. Lyon

DATE. Feb 88 (orig data); Feb 92 (modifications)

REFS. None

COMPOSITION. Ag

CODES. GRIZZLY

RANGE. 69 densities, 0., 1.05E-5, 2.1E-5, ..., 2.1E+5 g/cc,  
37 temperatures, 0., 145.1, 298.2, 580.2, ..., 1.16E9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give RREF=10.507, TREF=298.152, and BREF=94.162 GPa. The value of BREF corresponds to a sound speed of 3.0461 km/s.
- No changes were made to the 301 table.

#### COMMENTS.

- TFD as calculated by candide in GRIZZLY was used for the electronic contribution. Chartjd nuclear model with JD Gamma (igrun=7). Gamref=2.4, debkel=230, tmelt=1234, dgamma=(-4.0, -2.0), gameps=(0.667, 3.0). Cold curve from shock data. Us-up composed of one

straight line with  $c_0=3.27$  and  $s=1.55$ .  $CMAT=1.85$ ,  $ecohkc=68.0$ ,  $fac1j=0.195$ . 301 table has Van der Waals loops. Critical temperature is 4300K.

- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than 3660K.
- Pressure, energy and free energy are tabulated in the 301 table.
- A negative internal energy exists for temperatures less than TREFF.

#### EOS NUMBER 2961

MATERIAL. Titanium Alloy (Z=21.118, A=45.876)

SOURCE. J. Johnson, S. Lyon

DATE. July 85 (orig data); Feb 92 (modifications)

REFS. None

COMPOSITION. 90% Ti, 6% Al, 4% V by weight

CODES. GRIZZLY

RANGE. 72 densities, 0., 4.45E-6, 8.89E-6, ..., 8.89E4 g/cc,

37 temperatures, 0., 145.1, 298.2, 580.2, ..., 1.16E9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=4.4469, TREF=298.152, and BREF=10.6232 GPa. The value of BREF corresponds to a sound speed of 4.9121 km/s.
- No changes were made to the 301 table.

COMMENTS.

- Average atom modeling throughout. TFD as calculated by GRIZZLY was used for the electronic contribution. Chartjd nuclear model. Cold curve from shock data and sound velocity. Us-up composed of four straight lines ( $u_p=0.0, 0.58, 0.88, 1.66, 3.2$  and  $u_s=4.937, 5.72, 5.72, 6.65, 8.18$ ). TFD match made at compression of 1.64. ECOH=112 kcal per mole and FACLJ=1.0. Special gamma ( $ig\ run=7$ ) with  $gamref=1.3$ ,  $gameps=0.5, 1.0$  and  $dgamma=-0.8, -0.8$ . Debyeref=400 K.
- This EOS does not have Maxwell constructions. There is a tension region for temperatures less than approximately 7665K.
- Negative internal energy exists for temperatures less than TREFF.
- Pressure, energy and free energy are tabulated in the 301 table.

#### EOS NUMBER 2980

MATERIAL. Molybdenum (Z=42, A=95.940)

SOURCE. J. Barnes, J. Rood

DATE. Mar 73 (orig data); Feb 92 (modifications)

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Mo

CODES. Sesame I, Maple, Maxwell

RANGE. 101 densities, 0., 7.969E-2, 1.52E-1, ..., 2.04E+5 g/cc,

23 temperatures, 0., 290.12, 580.24, 1160.5, ..., 3.71E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=10.1756, TREF=290.121, and BREF=254.377 GPa. The value of BREF corresponds to a sound speed of 5.0127 km/s.
- In the tension region modifications were made to the 301 table at  $T<1160$  K and  $density<9.9033$  g/cc to make pressure proportional to density and energy constant.

COMMENTS.

- This EOS is quite old - use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- There is a tension region for temperatures below 1160K.
- This EOS is not thermodynamically consistent in the vapor-liquid region. Maxwell constructions were put into the pressure table but not in the energy table.
- Interpolation on the tables produces spurious cross-overs in the pressure isotherms for temperatures in the approximate range of  $1100 < T < 5840$ .
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 3100

MATERIAL. Nickel ( $Z=28$ ,  $A=58.710$ )

SOURCE. J. Barnes, J. Rood

DATE. Mar 73 (orig data); Feb 92 (modifications)

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Ni

CODES. Sesame I, Maple, Maxwell

RANGE. 101 densities,  $0., 6.939E-2, 1.324E-1, \dots, 1.776E+5$  g/cc,  
23 temperatures,  $0., 290.12, 580.24, 1160.5, \dots, 3.71E8$  Kelvin.

MODIFICATIONS.

- The 201 table was modified to give  $RREF=8.8235$ ,  $TREF=290.121$ , and  $BREF=183.477$  GPa. The value of BREF corresponds to a sound speed of 4.604 km/s.
- In the tension region modifications were made to the 301 table at  $T < 1160$  K and  $\text{density} < 8.151$  g/cc to make pressure proportional to density and energy constant.

COMMENTS.

- This EOS is quite old - use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- It has a tension region for temperatures less than 1160 K.
- Interpolation on the tables produces spurious cross-overs in the pressure isotherms for temperatures greater than about 1800K.
- This EOS is not thermodynamically consistent in the vapor-liquid region. Maxwell constructions were put into the pressure table but not in the energy table.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 3200

MATERIAL. Lead ( $Z=82$ ,  $A=207.19$ )

SOURCE. J. Barnes, J. Rood

DATE. Apr 75, Aug 78 (orig data); Feb 92 (modifications)

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Pb

CODES. Sesame I, Maple, Maxwell

RANGE. 101 densities,  $0., 8.86E-2, 0.169, \dots, 2.268E+5$  g/cc,  
23 temperatures,  $0., 290.12, 580.24, 1160.5, \dots, 3.71E8$  Kelvin.



## MODIFICATIONS.

- The 201 table was modified to give RREF=11.1591, TREF=290.121, and BREF=45.2869 GPa. The value of BREF corresponds to a sound speed of 2.0482 km/s.
- In the tension region modifications were made to the 301 table at  $T < 2307$  K and density  $< 9.0733$  g/cc to make pressure proportional to density and energy constant.

## COMMENTS.

- The tension region (for spall) was first added on 8-24-78 by Jerry Rood at the request of Mel Thieme (x-4). The tension region exists for temperatures below 2307K.
- This EOS is quite old - use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- This EOS is not thermodynamically consistent in the vapor-liquid region. Maxwell constructions were put into the pressure table but not in the energy table.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

## EOS NUMBER 3330

MATERIAL. Copper (Z=29.0, A=63.54)

SOURCE. J. Barnes, J. Rood

DATE. May 74

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Cu

CODES. SESAME I, MAPLE

RANGE. 101 densities, 0., 0.07, 0.13..., 1.8E+5 g/cc,  
23 temperatures, 0., 290.121, ..., 3.7E8 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give RREF=8.8433, TREF=290.121, and BREF=131.339 GPa. The value of BREF corresponds to a sound speed of 3.854 km/s.
- The low density-temperature region,  $\rho < 8.193$ ,  $t < 1200$  K, was modified to make pressure proportional to density and energy constant.

## COMMENTS.

- This EOS is quite old - use with caution. One deficiency is that the room temperature density has been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- It has a tension region for temperatures below about 2320 K.
- Only pressure and energy are tabulated in the 301 table. There is no entropy or free energy table.

## EOS NUMBER 3333

MATERIAL. Copper (Z=29.0, A=63.54)

SOURCE. K. Trainor

DATE. Feb. 84

REFS. K. S. Trainor, J. Appl. Phys. 54(5), 1983.

K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Cu

CODES. APW, ACTEX (F. Rogers, LLNL), OCCIPITAL (C. Rouse, LLNL),  
SOFTSPHERE (D. Young, LLNL), GRAY (R. Grover, LLNL),

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TFNUC (F. Ree, LLNL)

RANGE. 74 densities, 0.,1.E-6,...,1.E+3 g/cc,  
65 temperatures, 0.,299.976,...,5.8E8 Kelvin.

### MODIFICATIONS.

The 201 table was modified to give RREF=8.93, TREF=299.9763, and  
BREF=138.6 GPa. The value of BREF corresponds to a sound speed

### COMMENTS.

- EOS 3331, on which this EOS is based, is a global equation of state which ranges from densities of 1.0e-3 to 1.0e+3 gm per cc and from ambient temperature to 5.0e+4 eV. Six different theoretical models were used: a soft sphere liquid metal model at low temperatures below melt density; an ionization equilibrium model based on a modified Saha method at moderate temperatures in expansion; a nonideal plasma theory for high temperatures; a modified Thomas-Fermi-Kirzhnits model in compression; rigorous electron band theory for zero degree isotherm; and a semi-empirical model in the solid-liquid-vapor region. Agreement with existing experimental data (including soviet release isentrope data) is excellent.
- EOS 3333 is an extension of sesame 3331 downward in density from 1.0e-3 g/cc to 1.0e-6 g/cc. A Saha model was used for the extension at temperatures above 0.316 eV. Below that temperature, we used the soft sphere model for liquid metals developed by David Young at LLNL. In addition, a pseudo curve was added to the table by logarithmically extrapolating the pressures and energies down from the lowest two finite temperature isotherms. A zero density isochore was also put in -- the pressures were set to zero, and the energy was calculated by extrapolating down linearly from the two lowest density points in the table.
- A problem with this EOS is that it has no tension region, so it will not predict fracture in dynamic calculations. In addition, the interpolation scheme does not give the correct sound speed at ambient density and temperature.
- Only pressure and energy are tabulated in the 301 table. There is no entropy or free energy table.

### EOS NUMBER 3336

MATERIAL. Copper (Z=29.0, A=63.54)

SOURCE. K. Holian

DATE. Obtained from LANL in Mar 91

REFS. none

COMPOSITION. Cu

CODES.

RANGE. 74 densities, 0.,1.E-6,...,1.E+3 g/cc,  
65 temperatures, 0.,299.976,...,5.8E8 Kelvin.

### MODIFICATIONS.

The 201 table was modified to give RREF=8.93, TREF=299.9763, and  
BREF=143.975 GPa. The value of BREF corresponds to a sound speed

### COMMENTS.

- This EOS is like 3333 except that it has a tension region at low temperatures and densities near normal, for treatment of fracture in dynamic calculations. Interpolation on the table does give a reasonable value for the sound speed.
- Only pressure and energy are tabulated in the 301 table. There is no entropy or free energy table.

### EOS NUMBER 3520

MATERIAL. Tantalum (Z=73.0, A=180.948)  
 SOURCE. B. Bennett  
 DATE. Feb 83 (orig data); Feb 92 (modifications)  
 REFS. Hugdata, Sandia Laboratories Report SC-RR-70-28  
 COMPOSITION. Ta  
 CODES. EOSCRAY, CANDIDE  
 RANGE. 49 densities, 0., 1.68, 1.81, ..., 42.929 g/cc,  
 16 temperatures, 0., 298.12, 580.22, 870.34, ..., 6.526E5 Kelvin.  
 MODIFICATIONS.

- The 201 table was modified to give RREF=16.6540, TREF=298.12, and BREF=194.897 GPa. The value of BREF corresponds to a sound speed of 3.4338 km/s.
- No changes were made to the 301 table.

## COMMENTS.

- This EOS uses the chart-d form for gamma and the debye temperature for compressions greater than one and a virial match for compressions less than one. The thermal electronic model is Thomas-Fermi-Dirac with Kohn-Sham exchange. The cold curve is generated from a linear fit to the shock data (us vsup). As a result, the EOS reproduces the shock data to an accuracy of less than 0.4% over the range of the data. It is intended that this EOS be for applications under compression and not for vapor pressure calculations.
- This EOS has no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. (See above comment.) It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than 12,524K.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 3541

MATERIAL. Tungsten (Z=74.00000, A=183.85000)  
 SOURCE. B. Bennett  
 DATE. Sept 79  
 REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
 Los Alamos National Laboratory report LA-10160-MS, 1984  
 COMPOSITION. W  
 CODES. EOSLTS, CANDIDE  
 RANGE. 84 densities, 0., 1.9E-4, ..., 1.9E+4 g/cc,  
 25 temperatures, 0., 298.120, ..., 1.16E8 Kelvin.  
 MODIFICATIONS.

The 201 table was modified to give RREF=19.237, TREF=298.12, and BREF=311.312 GPa. The value of BREF corresponds to a sound speed of 4.0228 km/s.

## COMMENTS.

- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- Only pressure and energy are tabulated in the 301 table. There is no entropy or free energy table.

## EOS NUMBER 3542

MATERIAL. Tungsten alloy (Z=67.31600, A=165.78000)  
 SOURCE. K. Holian  
 DATE. received from LANL in Mar 91  
 REFS. See notes for EOS 3541

COMPOSITION. ?

CODES. See notes for EOS 3541

RANGE. 84 densities, 0.,1.7E-4,...,1.7E+4 g/cc,  
25 temperatures, 0.,298.120,...,1.16E8 Kelvin.

MODIFICATIONS.

The 201 table was modified to give RREF=17.346, TREF=298.12, and  
BREF=311.301 GPa. The value of BREF corresponds to a sound speed  
of 4.2363 km/s.

COMMENTS.

- This EOS has van der Waals loops and no Maxwell constructions.  
Hence it gives a tension region for use with fracture models but  
does not describe vaporization correctly. It does give the  
correct sound speed at the reference state.
- Only pressure and energy are tabulated in the 301 table. There is  
no entropy or free energy table.

EOS NUMBER 3560

MATERIAL. Tungsten Carbide (Z=38.75335311, A=94.19088602)

SOURCE. R. Albers

DATE. Nov 81 (orig data); Feb 92 (modifications)

REFS. None

COMPOSITION. WC with trace of Co - 88.235%W 5.765%C 6%Co (by weight)

CODES. TFD, EOS0422

RANGE. 100 densities, 0.,1.5E-4,1.8E-4,...,1.5E4 g/cc,  
25 temperatures, 0.,298.12,580.23,1160.45,...,3.48E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=14.9699, TREF=298.12,  
and BREF=359.30 GPa. The value of BREF corresponds to a sound  
speed of 4.911 km/s.
- No changes were made to the 301 table.

COMMENTS.

- The author warns: "When comparing to experimental shock data, note  
that low pressure data is bad because of fast longitudinal sound  
waves closing gaps before the shock wave arrives."
- This EOS does not have Maxwell constructions. There is a tension  
region for temperatures less than 13,350 K. Vaporization is not  
described correctly.
- The correct sound speed at the reference state needs to be checked (ok  
by  $\text{SQRT}(\text{bref}/\text{ref})$ ).
- Pressure, energy and free energy are tabulated in the 301 table.

EOS NUMBER 3715

MATERIAL. Aluminum (Z=13.0, A=26.9815)

SOURCE. Kathy Trainor

DATE. DEC 83

REFS. K. S. Trainor, "A New Full-Range Equation of State for Aluminum",  
in H-Division Quarterly Report (April through June, 1982),  
Lawrence Livermore National Laboratory Report UCID-118574-82-2  
(1982), p.20.

K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Al

CODES. APW, ACTEX (F. Rogers, LLNL), OCCIPITAL (C. Rouse, LLNL),  
SOFTSPHERE (David Young, LLNL), GRAY (R. Grover, LLNL),  
Pseudopotential code from Marvin Ross, LLNL.

RANGE. 100 densities, 0.,1.E-6,...,1.E+3 g/cc,

53 temperatures, 0.,299.976,...,1.2E8 Kelvin.

#### MODIFICATIONS.

The 201 table was modified to give RREF=2.70, TREF=299.9763, and BREF=77.28 GPa. The value of BREF corresponds to a sound speed of 5.35 km/s.

#### COMMENTS.

- EOS 3712, on which this EOS is based, is a global equation of state which ranges from densities of 1.0e-3 to 1.0e+3 gm per cc and from ambient temperature to 5.0e+4 eV. Seven different theoretical models were used: a soft sphere liquid metal model at low temperatures below melt density; an ionization equilibrium model based on a modified Saha method at moderate temperature in expansion; a nonideal plasma theory for high temperatures; a Thomas-Fermi-kirzhnits model corrected for thermal ion contributions in compression; rigorous electron band theory for the zero degree isotherm; a semi-empirical model in the solid-liquid-vapor region; and liquid metal perturbation theory based on pseudopotentials for the hot, dense, partially ionized liquid. Agreement with existing experimental data is excellent.
- EOS table 3715 is an extension of Sesame 3712 downward in density from 1.0e-3 g/cc to 1.0e-6 g/cc. A Saha model was used for the extension at temperatures above 0.4 eV, and the soft sphere model for liquid metals, developed by Dave Young at LLNL was used at the lower temperatures. In addition, a pseudo cold curve was added to the table by logarithmically extrapolating the pressures and energies down from the lowest two finite temperature isotherms. A zero density isochore was also put in -- the pressures were set to zero and the energy was calculated by extrapolating down linearly from the two lowest density points in the table.
- A problem with this EOS is that it has no tension region, so it will not predict fracture in dynamic calculations. In addition, the interpolation scheme does not give the correct sound speed at ambient density and temperature.
- Only pressure and energy are tabulated in the 301 table. There is no entropy or free energy table.

#### EOS NUMBER 3730

MATERIAL. Platinum (Z=78, A=195.09)

SOURCE. J. Barnes, J. Rood

DATE. Oct 72 (orig data); Feb 92 (modifications)

REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984

COMPOSITION. Pt

CODES. Sesame I, Maple, Maxwell

RANGE. 101 densities, 0.,0.167,0.319,...,2.142E4 g/cc,

23 temperatures, 0.,290.121,580.24,1160.48,...,3.71E8 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give RREF=21.329, TREF=290.121, and BREF=274.798 GPa. The value of BREF corresponds to a sound speed of 3.6078 km/s.
- In the tension region modifications were made to the 301 table at T<2330 K and density<18.725 g/cc to make pressure proportional to density and energy constant.

#### COMMENTS.

- This EOS is quite old - use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.121

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- even though it does not give the correct density.
- There is a tension region for temperatures below 2330 K.
- This EOS is not thermodynamically consistent in the vapor-liquid region. Maxwell constructions were put into the pressure table but not in the energy table.
- Interpolation on the tables produces spurious cross-overs in the pressure isotherms for temperatures in the approximate range of  $1500 < T < 2740$ .
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

### EOS NUMBER 4100

MATERIAL. Brass ( $Z=29.777$ ,  $A=65.334$ )  
SOURCE. J. Barnes, A. Lindstrom  
DATE. May 76, Aug 78 (orig data); Feb 92 (modifications)  
REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984  
COMPOSITION. Cu (61.5%) Zn (36%) Pb (2.5%) by weight  
CODES. Sesame I, Maple, Maxwell, Mod-Morse  
RANGE. 101 densities, 0.,  $6.6E-2$ ,  $0.126$ , ...,  $1.69E5$  g/cc,  
23 temperatures, 0.,  $290.121$ ,  $580.24$ ,  $1160.48$ , ...,  $3.71E8$  Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give  $RREF=8.32913$ ,  $TREF=290.121$ , and  $BREF=92.886$  GPa. The value of BREF corresponds to a sound speed of  $3.4129$  km/s.
- In the tension region modifications were made to the 301 table at  $T < 1500$  K and density  $< 7.464$  g/cc to make pressure proportional to density and energy constant. A  $\rho=0.0$  isochore was added to the 301 table.

#### COMMENTS.

- The tension region (for spall) was first added on 8-24-78 by Jerry Rood at the request of Mel Thieme (X-4). The tension region exists for temperatures below 2320 K.
- This EOS is quite old and should be used with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

### EOS NUMBER 4270

MATERIAL. Stainless Steel ( $Z=25.802$ ,  $A=55.365$ )  
SOURCE. A. Lindstrom  
DATE. Apr 76  
REFS. K. S. Holian, "T-4 Handbook of Material Properties Data Bases,"  
Los Alamos National Laboratory report LA-10160-MS, 1984  
COMPOSITION. 70.0 wt% Fe, 19.0 wt% Cr, 11.0 wt% Ni  
CODES. SESAME I, MAPLE, MAXWELL  
RANGE. 101 densities, 0.,  $6.2E-2$ ,  $0.118$ , ...,  $1.6E+5$  g/cc,  
23 temperatures, 0.,  $290.121$ , ...,  $3.7E8$  Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give  $RREF=7.8422$ ,  $TREF=290.121$ , and  $BREF=160.893$  GPa. The value of BREF corresponds to a sound speed of  $4.529$  km/s.
- A  $\rho=0$  isochore was added to the table.
- The low density-temperature region,  $\rho < 7.244$ ,  $t < 1200$ K, was modified

to make pressure proportional to density and energy constant.  
COMMENTS.

- This EOS is quite old - use with caution. One deficiency is that the room temperature density has been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- Another problem is that the lowest density is quite high, 0.06 g/cc.
- It has a tension region for temperatures below about 2320 K.
- Only pressure and energy are tabulated in the 301 table. There is no entropy or free energy table.

## EOS NUMBER 5000

MATERIAL. Nitrogen (Z=7, A=14.0067)

SOURCE. G. Kerley, J. Abdallah

DATE. Apr 81, Feb 83 (orig data); Mar 92 (modifications)

REFS. JCP 73, 5337 (1980)

COMPOSITION. N2

CODES. PANDA (no dissociation or electronic terms included)  
TUTTI code used to add the solid region.

RANGE. 64 densities, 0., 1.0E-8, 3.16E-8, ..., 1.0E4 g/cc,  
26 temperatures, 0., 31.57, 63.15, 100, ..., 1.0E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=0.857226 g/cc, TREFF=63.148K, PREF=1.2464E-5 GPa and BREF=0.358256 GPa (triple point values from SESAME 5001). The value of BREF corresponds to a sound speed of 0.86262 km/s.
- A rho=0.0 isochore was added to the 301 table.

COMMENTS.

- This EOS was constructed for the molecular species only and is not valid in regions where dissociation is important, at temperatures above 10,000K or pressures above 30 GPa. Data points are included outside the range of validity to prevent extrapolation problems. The 301 table was replaced (Feb 83) to correct low-temperature high-density crossing isotherms.
- This EOS does not have Maxwell constructions.
- It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than 115K.
- A negative internal energy exists for temperatures less than TREFF.
- This EOS is quite old and should be used with caution.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 5010

MATERIAL. Oxygen (Z=8, A=16)

SOURCE. G. Kerley, J. Abdallah

DATE. Apr 81, Feb 83 (orig data); Mar 92 (modifications)

REFS. JCP 73, 5337 (1980)

COMPOSITION. O2

CODES. PANDA (no dissociation or electronic terms included)  
TUTTI code was used to add the solid region.

RANGE. 64 densities, 0., 1.0E-8, 3.16E-8, ..., 1.0E4 g/cc,  
26 temperatures, 0., 31.57, 63.15, 100, ..., 1.0E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=1.26205 g/cc, TREFF=54.38K, PREF=1.49E-7 GPa and BREF=0.804836 GPa (triple point values from SESAME 5011). The value of BREF corresponds to a sound speed of 1.0361 km/s.

- A  $\rho=0.0$  isochore was added to the 301 table.

COMMENTS.

- This EOS was constructed for the molecular species only and is not valid in regions where dissociation is important, at temperatures above 10,000K or pressures above 30 GPa. Data points are included outside the range of validity to prevent extrapolation problems. The 301 table was replaced (Feb 83) to correct low-temperature high-density crossing isotherms.
- This EOS does not have Maxwell constructions.
- It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than 140K.
- A negative internal energy exists for temperatures less than TREFF.
- This EOS is quite old and should be used with caution.
- Pressure, energy and free energy are tabulated in the 301 table.

EOS NUMBER 5030

MATERIAL. Dry Air ( $Z=7.37296$ ,  $A=14.80304$ )

SOURCE. H. C. Graboske

DATE. Dec 81 (orig data); Mar 92 (modifications)

REFS. UCID-16901

COMPOSITION. N2[78.09%] O2[21.95%] Ar[0.96%]

CODES. see UCID-16901

RANGE. 22 densities, 0., 1.0E-7, 5.5E-7, ..., 15 g/cc,  
32 temperatures, 0., 175.24, 958, 1740.75, ..., 3.48E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give TREF=298 K, PREF=1.013E-4 GPa (STP Conditions), RREF=1.21798E-3 g/cc and BREF=1.00998E-4 GPa. The value of BREF corresponds to a sound speed of 0.33882 km/s.
- A  $\rho=0.0$  isochore and  $T=0.0$  isotherm were added to the 301 table.

COMMENTS.

- Zero pressures do not exist in the 301 table.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 5172

MATERIAL. Argon ( $Z=18$ ,  $A=39.948$ )

SOURCE. J. Wolford (LLNL), K. Trainor

DATE. Jan 83 (orig data); Mar 92 (modifications)

REFS. J. Wolford and K. Long, "A New Theoretical EOS for Argon," in H-Division Quarterly Report UCID-18574-81-3, Lawrence Livermore National Laboratory, Livermore CA 94550 (1981)

COMPOSITION. Ar

CODES. OCCIPITAL (SAHA), ACTEX (Quantum Statistical Mechanical Based on Perturbation Theory), TFNUC (Thomas-Fermi Plus Nuclear Corrections), LMTO, LNJ (Lennard-Jones 6-12), and EXPERT (Exponential-Six Fluid Perturbation Theory).

RANGE. 67 densities, 0., 1.0E-5, 1.6E-5, ..., 1000.0 g/cc,  
59 temperatures, 0., 83.8, 116.04, 145.05, ..., 1.16E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=1.40746 g/cc, TREF=83.8 K, PREF=6.89E-5 GPa and BREF=0.615291 GPa, all corresponding to values at the triple point (from SESAME 5171). BREF corresponds to a sound speed of 0.86381 km/s.
- A  $\rho=0.0$  isochore, and  $T=0.0$  and 83.8 isotherms were added to the 301 table.

COMMENTS.



- The equation of state for argon is a global EOS which extends from .001 to 1.e+4 ev in temperature and from 1.e-5 to 1.e+3 gm/cc in density. This EOS incorporates the physics of six different theoretical models: (1) a Saha model for the ideal gas, ideal plasma and part of the ionization equilibrium regime; (2) a nonideal, quantum-statistical-mechanical theory for most of the ionization equilibrium regime; (3) a Thomas-Fermi-Kirzhnits model corrected for thermal ion contributions in compression; (4) electron band theory embodied in a linear muffin tin orbital (LMTO) code for the zero degree isotherm; (5) an exponential-six fluid perturbation theory for the high density fluid; and (6) an analytic fit to the Lennard-Jones 6-12 equation of state for the neutral fluid region. Favorable comparisons exist with the following experimental data: critical point data; soviet low-pressure p-v-t data; static high pressure data; soviet shock tube data; and Hugoniot data.
- This EOS does not have a zero pressure point.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

## EOS NUMBER 5181

MATERIAL. Krypton (Z=36, A=83.8)

SOURCE. G. Kerley

DATE. Nov 83 (orig data); Mar 92 (modifications)

REFS. LA-8062

COMPOSITION. Kr

CODES. PANDA, INFERNO, ERMA, TUTTIUSES

RANGE. 73 densities, 0., 1.0E-8, 1.0E-7, ..., 1.0E4 g/cc,  
 37 temperatures, 0., 38.6, 77.2, 115.8, ..., 4.0E8 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give RREF=2.49008 g/cc, TREF=115.8K, PREF=0.0 GPa and BREF=0.0957749 GPa (TREF corresponds to the melting temperature). The value of BREF corresponds to a sound speed of 0.57223 km/s.
- A rho=0.0 isochore was added to the 301 table.

## COMMENTS.

- The fluid model described in LA-8062, but with an improved model of the thermal electronic term. The Saha theory was used for densities below the metallic transition, and INFERNO was used above, with a region of interpolation from 3.2 to 17.0 g/cc. Both solid and fluid phases are included.
- This EOS does not have Maxwell constructions. Hence it gives a tension region for temperatures less than 197K but does not describe vaporization correctly.
- Pressure, energy and free energy are tabulated in the 301 table.
- A negative internal energy exists for temperatures less than TREF.

## EOS NUMBER 5190

MATERIAL. Xenon (Z=54, A=131.3)

SOURCE. G. Kerley

DATE. Nov 83 (orig data); Sep 92 (modifications)

REFS. LA-8062

COMPOSITION. Xe

CODES. PANDA, INFERNO, ERMA, TUTTI

RANGE. 67 densities, 0.0, 1.0e-6, ..., 5000 g/cc,  
 35 temperatures, 0.0, 53.8, 107.6, ..., 4.0e8 Kelvin.

## MODIFICATIONS.

## Sandia EOS Data Base

- The 201 table was modified to give  $PREF=1.013e-4$  GPa,  $TREF=298.15$  K [STP Conditions],  $RREF=0.005391$  g/cc and  $BREF=1.00879e-4$  GPa. The value of BREF corresponds to a sound speed of 0.17697 km/s.
- A  $\rho=0.0$  isochore and  $T=298.15$  isotherm were added to the 301 table.

### COMMENTS.

- Uses the fluid model described in LA-8062, but with a cold curve based on calculations of McMahan and Ross, and with an improved model of the thermal electronic term. The Saha theory was used for densities below the metallic transition, and Inferno was used above, with a region of interpolation from 4.6 to 40.0 g per cc. Gives good agreement with the softening of the hughoniot observed by Nellis, et. al. Both solid and fluid phases are included.
- There are no Maxwell constructions in the vaporization region.
- This EOS is quite old so use with caution.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 5251

MATERIAL. Hydrogen ( $Z=1$ ,  $A=1.00797$ )

SOURCE. R. Albers, J. Johnson

DATE. Sep 82 (orig data); Sep 92 (modifications)

REFS. Memo dated 9-27-82 by R. Albers and J. Johnson

COMPOSITION. Natural mix of hydrogen isotopes

CODES. FIXTAB3

RANGE. 50 densities, 0.0, 5.0e-6, ..., 1751.7 g/cc,  
25 temperatures, 0.0, 290.0, 477.2, ..., 3.7e8 Kelvin.

### MODIFICATIONS.

- The 201 table was modified to give  $PREF=0.31349$  GPa,  $TREF=298.15$  K,  $RREF=0.088385$  g/cc and  $BREF=0.76059$  GPa. The value of BREF corresponds to a sound speed of 3.328 km/s.

### COMMENTS.

- This is an isotope scaling of the corrected 5263 tables (9-27-82) to produce h2 (natural mix) tables.
- There are no Maxwell constructions in the vaporization region.
- This EOS is quite old so use with caution.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

### EOS NUMBER 5263

MATERIAL. Deuterium ( $Z=1.0$ ,  $A=2.014$ )

SOURCE. G. Kerley

DATE. Oct 71 (rerun Sep 74) (orig data); Sep 92 (modifications)

REFS. LA-4760, LA-4776

COMPOSITION. D2

CODES. D2EOS

RANGE. 50 densities, 0.0, 1.0e-5, ..., 3500 g/cc,  
25 temperatures, 0.0, 290.0, 477.2, ..., 3.7e8 Kelvin.

### MODIFICATIONS.

- The 201 table was modified to give  $PREF=0.31349$  GPa,  $TREF=298.15$  K,  $RREF=0.1766$  g/cc and  $BREF=0.76059$  GPa. The value of BREF corresponds to a sound speed of 2.3544 km/s.

### COMMENTS.

- A 3-phase eos (fluid, molecular solid, metallic solid). Fluid includes dissociation and ionization. Good agreement with Las1 and 111 shock data and with static data for liquid to 20 kbar.

Metallic transition at 2.2 mbar agrees with 111 experiment (Phys. Rev. Lett., v41, p994). Ion table added on 12 aug 80. We have updated the existing 5263 using code Fixtab3. The only change involved replacing one point in the energy of the 301 and 303 tables. This energy point at  $t = 5.192e4$  kelvin and  $\rho = 609.4$  gm per cc was changed by about 1% to prevent a negative specific heat. For further information, see memo dated 9-27-82 by R Albers and J. Johnson.

- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

## EOS NUMBER 5410

MATERIAL. Neon ( $Z=10$ ,  $A=20.183$ )

SOURCE. J. Barnes, J. Rood

DATE. Nov 75 (orig data); Sep 92 (modifications)

REFS. none

COMPOSITION. Ne

CODES. SESAME I

RANGE. 101 densities, 0.0, 0.013, ..., 28800 g/cc,

23 temperatures, 0.0, 290.12, 580.2, ..., 3.7e8 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give  $PREF=0.37998$  GPa,  $TREF=290.12$  K,  $RREF=1.44$  g/cc and  $BREF=1.40515$  GPa. The value of BREF corresponds to a sound speed of 1.0944 km/s.

## COMMENTS.

- There are Maxwell constructions in the vaporization region.
- This EOS does not have a tension region.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

## EOS NUMBER 5500

MATERIAL. Methane ( $Z=2$ ,  $A=3.20852$ )

SOURCE. G. Kerley

DATE. Jan 80 (orig data); Sep 92 (modifications)

REFS. Publication in preparation

COMPOSITION. CH4

CODES. PANDA, TUTTI

RANGE. 70 densities, 0.0, 1.0e-10, ..., 2.5 g/cc,

23 temperatures, 0.0, 20.0, 45.0, ..., 10000 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give  $PREF=1.013e-4$  GPa,  $TREF=95$  K [ Approximate Triple Point],  $RREF=0.42634$  g/cc and  $BREF=0.0231175$  GPa. The value of BREF corresponds to a sound speed of 0.2429 km/s. A  $\rho=0.0$  isochore and  $T=0.0$  isotherm were added to the 301 table.

## COMMENTS.

- Equilibrium eos table, has Maxwell constructions. 401 table (vaporization) included. Good agreement with experiment except near critical point.
- Since this EOS was constructed for the molecular species only, it is not valid in regions where dissociation is important, i.e. above 5,000 degrees Kelvin. Isotherms are included above this temperature to prevent extrapolation problems.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 5760

MATERIAL. Helium (Z=2, A=4.0026)  
 SOURCE. Lawrence Livermore Laboratory  
 DATE. Aug 74 (orig data); Sep 92 (modifications)  
 REFS. UCIR-740  
 COMPOSITION. He-4  
 CODES. See UCIR-740  
 RANGE. 101 densities, 0.0,1.8e-3,...,4678.4 g/cc,  
 25 temperatures, 0.0,116,298.15,...,1.16e8 Kelvin.  
 MODIFICATIONS.  
 - The 201 table was modified to give PREF=0.28858 GPa, TREF=298.15K,  
 RREF=0.23392 g/cc and BREF=0.555593 GPa. The value of BREF  
 corresponds to a sound speed of 1.8601 km/s. A T=298.15 isotherm  
 was added to the 301 table.  
 COMMENTS.  
 - There are no Maxwell constructions in the vaporization region.  
 - Only pressure and energy are tabulated in the 301 table. Entropy  
 and free energy are not included.

EOS NUMBER 5761

MATERIAL. Helium (Z=2, A=4.0026)  
 SOURCE. R. Albers  
 DATE. Mar 81 (orig data); Sep 92 (modifications)  
 REFS. None  
 COMPOSITION. He-4  
 CODES. PANDA (specially modified version)  
 RANGE. 38 densities, 0.0,1.0e-6,...,1000 g/cc,  
 27 temperatures, 0.0,6,12,...,1.16e8 Kelvin.  
 MODIFICATIONS.  
 - The 201 table was modified to give PREF=1.0713 GPa,  
 TREF=298.15 K, RREF=0.4 g/cc and BREF=2.54946 GPa.  
 The value of BREF corresponds to a sound speed of 2.9029 km/s.  
 COMMENTS.  
 - This EOS is quite old so use with caution.  
 - There are no Maxwell constructions in the vaporization region.  
 - This EOS does not have a tension region.  
 - Only pressure and energy are tabulated in the 301 table. Entropy  
 and free energy are not included.

EOS NUMBER 7100

MATERIAL. Dry Sand (Z=9.549, A=19.124)  
 SOURCE. J. Barnes, S. Lyon  
 DATE. June 87 (orig data); Mar 92 (modifications)  
 REFS. None  
 COMPOSITION. SiO2[70%] Al2O3[8.22%] CaO[4.25%] Fe2O3[4.53%]  
 CO2[3.87%] H2O[3.02%] K2O[2.06%] MgO[1.89%] SO3[0.69%]  
 TiO2[0.58%] Na2O[0.58%] by weight  
 CODES. GRIZZLY  
 RANGE. 73 densities, 0.,2.6E-6,5.2E-6,...,5.2E4 g/cc,  
 37 temperatures, 0.,145.06,298.15,580.24,...,1.16E9 Kelvin.  
 MODIFICATIONS.  
 - The 201 table was modified to give RREF=2.60462, TREF=298.152,  
 and BREF=38.8555 GPa. The value of BREF corresponds to a  
 sound speed of 3.8831 km/s.  
 - No changes were made to the 301 table.  
 COMMENTS.  
 - Average atom modeling used throughout except for ideal gas portion

of nuclear model where ideal mixing was used. TFD as calculated by candide in GRIZZLY was used for the electronic contribution. Chartjd nuclear model with jd gamma (igrun = 7). Gamref = 0.875, gameps = (0.5,1.0), dgamma = (1.227,0.0), debkel = 849.4, tmelt = 0. In order to obtain the cold curve, the 5 major components of the sand (including water of hydration), were mixed in their relative ammounts using ideal mixing to produce a characteristic hugoniot. The us-up points taken from this curve were then (up,us) = (0.0,3.875), (0.774,5.375), (1.786,5.813), (2.524,6.375), (4.00,8.750). Cmat = 1.85, ecohkc = 136.7, fac1j = 0.25. 301table has van der Waals loops. Critical temperature is 8500 k.

- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than 8050K.
- Pressure, energy and free energy are tabulated in the 301 table.
- A negative internal energy exists for temperatures less than TREFF.

#### EOS NUMBER 7102

MATERIAL. Dry Clay (Z=9.154, A=18.312)

SOURCE. J. Barnes, S. Lyon

DATE. June 87 (orig data); Mar 92 (modifications)

REFS. None

COMPOSITION. SiO2[50.65%] Al2O3[15.1%] Cao[7.19%]

Fe2O3[6.47%] CO2[6.1%] H2O[5.58%] K2O[3.49%] MgO[3.31%]

Na2O3[0.81%] TiO2[0.78%] SO3[0.63%] by weight

CODES. GRIZZLY

RANGE. 71 densities, 0.,3.02E-6,6.03E-6,...,6.04E4 g/cc,

37 temperatures, 0.,145.06,298.15,580.24,...,1.16E9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=3.01647, TREF=298.152, and BREF=55.2552 GPa. The value of BREF corresponds to a sound speed of 4.3123 km/s.
- No changes were made to the 301 table.

COMMENTS.

- Average atom modeling used throughout except for ideal gas portion of nuclear model where ideal mixing was used. TFD as calculated by candide in GRIZZLY was used for the electronic contibution. Chartjd nuclear model with JD Gamma (igrun = 1). Gamref = 1.055, debkel = 766.9, tmelt = 0. In order to obtain the cold curve, the 5 major components of the clay (including water of hydration) were mixed in their relative ammounts to produce a characteristic hugoniot. The us-up point taken from this curve were then (up,us) = (0.0,4.33), (2.10,7.14), (3.18,9.00). Cmat = 1.55, ecohkc = 129, fac1j = 0.20. 301 table has van der Waals loops. Critical temperature is 6800 k.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than 6270K.
- Pressure, energy and free energy are tabulated in the 301 table.
- A negative internal energy exists for temperatures less than TREFF.

#### EOS NUMBER 7111

MATERIAL. Nevada Alluvium (Z=9.3659, A=18.761)

SOURCE. J. Barnes, J. Rood

DATE. Sept 75 (orig data); Mar 92 (modifications)

## Sandia EOS Data Base

REFS. None

COMPOSITION. SiO2[71.6%] Al2O3[12.1%] H2O[4.0%] K2O[3.5%] CaO[2.4%]  
by weight, plus lesser amounts of other oxides

CODES. SESAME I

RANGE. 101 densities, 0., 1.84E-2, 3.5E-2, ..., 4.7E4 g/cc,  
23 temperatures, 0., 290.12, 580.24, 1160.48, ..., 3.71E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=1.31285, TREF=290.121, and BREF=7.158 GPa. The value of BREF corresponds to a sound speed of about 2.335 km/s.
- A rho=0.0 isochore was added to the 301 table.

COMMENTS.

- This EOS is quite old, so use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- A problem with this EOS is that it has no tension region, so it will not predict fracture in dynamic calculations. In addition, the interpolation scheme does not give the correct sound speed at the reference state.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 7120

MATERIAL. Saturated Tuff (Z=6.83, A=13.4)

SOURCE. J. Johnson, S. Lyon

DATE. May 85 (orig data); Jun 92 (modifications)

REFS. None

COMPOSITION. SiO2[63.5%] H2O[21.3%] Al2O3[15.2%] by weight

CODES. GRIZZLY

RANGE. 75 densities, 0.0, 1.95E-6, ..., 3.9E+4 g/cc,  
37 temperatures, 0.0, 145.06, 298.152, ..., 1.16E+9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=1.94981 g/cc and BREF=9.94758 GPa. The value of BREF corresponds to a sound speed of 2.415 km/s.
- No changes were made to the 301 table.

COMMENTS.

- This EOS is for tuff with all voids filled with water. The void volume is 30% of the total volume. Note that even dry tuff has some water content. Average atom modeling throughout.
- TFD as calculated by GRIZZLY was used for the electronic contribution. Cold curve from shock data and sound velocity. Us-up composed of three straight lines (up = 0.0, 1.2, 2.53, 6.6 and us = 2.4, 4.3, 5.55, 12.13). Data from Eilers (private communication) for up = 0.0 and Isbell and Rosenberg et al for the remaining shock data. TFD match made at compression of 2.16. ecoh = 100 kcal per mole and fac1j = 0.23. Special gamma (igrun = 7) with gamref = 1.27, gameps = 0.5, 1.0 and dgamma = 1.377, 1.377. This gamref was picked between 2s-1 and the gamref of glass. Debyeref = 500 kelvin(a guess).
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than ~4000 K.

- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7121

MATERIAL. Saturated Tuff (Z=6.83, A=13.4)  
 SOURCE. J. Johnson, S. Lyon  
 DATE. May 85 (orig data); Jun 92 (modifications)  
 REFS. None  
 COMPOSITION. SiO<sub>2</sub>[63.5%] H<sub>2</sub>O[21.3%] Al<sub>2</sub>O<sub>3</sub>[15.2%] by weight  
 CODES. GRIZZLY  
 RANGE. 79 densities, 0.0, 1.95E-6, ..., 3.9E+4 g/cc,  
 37 temperatures, 0.0, 145.06, 298.152, ..., 1.16E+9 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=1.94946 g/cc and BREF=7.40064 GPa. The value of BREF corresponds to a sound speed of 2.0411 km/s.
- No changes were made to the 301 table.

## COMMENTS.

- This is the same as 7120 with the following changes: gamref = 0.9, dgamma = (-0.3, -0.3), cmat = 2.19, (up, us) = (0.0, 1.99), (0.4, 2.81), (0.7, 3.20), (1.5, 3.96), (2.15, 4.50), (4.0, 7.56), (6.6, 12.15).
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than ~4000K.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7130

MATERIAL. Limestone (Z=9.595, A=19.194)  
 SOURCE. J. Barnes, S. Lyon  
 DATE. Jan 88 (orig data); Jun 92 (modifications)  
 REFS. None  
 COMPOSITION. CaCO<sub>3</sub>[67.5%] SiO<sub>2</sub>[23.6%] Al<sub>2</sub>O<sub>3</sub>[7.0%]  
 H<sub>2</sub>O[1.9%] by weight  
 CODES. GRIZZLY  
 RANGE. 72 densities, 0.0, 2.74E-6, ..., 5.48E+4 g/cc,  
 37 temperatures, 0.0, 145.06, 298.152, ..., 1.16E+9 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.7410 g/cc and BREF=65.1092 GPa. The value of BREF corresponds to a sound speed of 4.8983 km/s.
- No changes were made to the 301 table.

## COMMENTS.

- This table was constructed using ideal mixing in GRIZZLY. The mixture consists of 67.5% caco3 (7331), 23.6% sio2 (7385), 7.0% al2o3 (7411), 1.9% h2o (7153) by weight. The 301 table was rescaled to a density of 2.741 and has Van der Waals loops. Critical temperature is 9900K.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than ~7850K.
- Pressure, energy and free energy are tabulated in the 301 table.

## Sandia EOS Data Base

### EOS NUMBER 7150

MATERIAL. Water ( $Z=3.3333$ ,  $A=6.0053$ )

SOURCE. F. H. Ree (Livermore)

DATE. Jun 77 Jan 78 (orig data); Mar 92 (modifications)

REFS. UCRL-7118; F. H. Ree, "Equation of State of Water," Lawrence Livermore Laboratory Report UCRL-52190 (Dec 76)

COMPOSITION. H<sub>2</sub>O

CODES. See Refs.

RANGE. 81 densities, 0.,  $2.0E-6$ ,  $2.5E-6$ , ..., 400 g/cc,  
45 temperatures, 0., 290.121, 348.15, 406.17, ...,  $1.74E8$  Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give  $PREF=0.0001013$ ,  $RREF=1.00001$ ,  $TREF=290.121$ , and  $BREF=1.38433$  GPa.  $BREF$  corresponds to a sound speed of 1.1794 km/s.
- A  $\rho=0.0$  isochore and  $T=0.0$  isotherm were added to the 301 table.

#### COMMENTS.

- The mesh for this EOS is rather coarse in some regions. It does not give a good representation of the vapor-liquid region.
- It does not have any zero pressure point or tension region.
- The sound speed at the reference state is not correct.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

### EOS NUMBER 7160

MATERIAL. Deutero-Polyethylene ( $Z=2.6666667$ ,  $A=5.3468$ )

SOURCE. F. Dowell

DATE. Sep 82 (orig data); Sep 92 (modifications)

REFS. LANL report to be published

COMPOSITION. CD<sub>2</sub>

CODES. FIXTAB3

RANGE. 65 densities, 0.0,  $1.05e-4$ , ..., 2094.9 g/cc,  
32 temperatures, 0.0, 100, 200, ...,  $1.16e9$  Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give  $PREF=0.0$  GPa,  $TREF=298.15$  K (STP conditions),  $RREF=1.0475$  g/cc and  $BREF=5.60381$  GPa. The value of  $BREF$  corresponds to a sound speed of 2.3975 km/s.
- No changes were made to the 301 table.

#### COMMENTS.

- This eos was created from 7171 by isotopic scaling.
- This EOS does not have Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than 560K.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 7171

MATERIAL. Polyethylene (branched) ( $Z=2.6666667$ ,  $A=4.6757$ )

SOURCE. F. Dowell

DATE. Sep 82 (orig data); Sep 92 (modifications)

REFS. LA-9559-MS

COMPOSITION. CH<sub>2</sub>

CODES. CANDIDE, PANDA

RANGE. 65 densities, 0.0,  $9.16e-5$ , ..., 1832 g/cc,  
32 temperatures, 0.0, 100, 200, ...,  $1.16e9$  Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give  $PREF=0.0$  GPa,  $TREF=298.15$  K



(STP conditions), RREF=0.91598 g/cc and BREF=5.60223 GPa. The value of BREF corresponds to a sound speed of 2.5632 km/s.

- No changes were made to the 301 table.

#### COMMENTS.

- This EOS does not have Maxwell constructions.  
Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than 560K.
- Pressure, energy and free energy are tabulated in the 301 table.

#### EOS NUMBER 7180

MATERIAL. Polyethylene (marlex) (Z=2.6666667, A=4.6757)

SOURCE. F. Dowell

DATE. Sep 82 (orig data); Sep 92 (modifications)

REFS. LA-9564-MS

COMPOSITION. CH2

CODES. CANDIDE, PANDA

RANGE. 65 densities, 0.0, 9.54e-5, ..., 1908 g/cc,

32 temperatures, 0.0, 100, 200, ..., 1.16e9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.15 K (STP conditions), RREF=0.95399 g/cc and BREF=6.76696 GPa. The value of BREF corresponds to a sound speed of 2.8016 km/s.
- No changes were made to the 301 table.

#### COMMENTS.

- This EOS does not have Maxwell constructions.  
Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than 560K.
- Pressure, energy and free energy are tabulated in the 301 table.

#### EOS NUMBER 7230

MATERIAL. Polytetradeuteroethylene (Z=2.6667, A=5.3469)

SOURCE. F. Dowell

DATE. Aug 84 (orig data); Sep 92 (modifications)

REFS. LA-10241-MS

COMPOSITION. CD2

CODES. GRIZZLY, FIXTAB

RANGE. 65 densities, 0.0, 1.09e-6, ..., 2186.0 g/cc,

33 temperatures, 0.0, 100, 200, ..., 1.16e9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.15 K (STP conditions), RREF=1.0925 g/cc and BREF=6.28365 GPa. The value of BREF corresponds to a sound speed of 2.4358 km/s.
- No changes were made to the 301 table.

#### COMMENTS.

- This EOS does not have Maxwell constructions.  
Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than 560K.
- Pressure, energy and free energy are tabulated in the 301 table.

#### EOS NUMBER 7190

MATERIAL. Teflon (Z=8, A=16.66927)

SOURCE. F. Dowell, J. Johnson

DATE. Aug 82 (orig data); Jul 92 (modifications)

## Sandia EOS Data Base

REFS. LA-9439-MS

COMPOSITION. CF<sub>2</sub>

CODES. CANDIDE, PANDA

RANGE. 64 densities, 0.0, 2.15E-3, ..., 4304 g/cc,  
32 temperatures, 0.0, 100, 200, ..., 1.16E9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.15 K (STP conditions), RREF=2.152 g/cc and BREF=5.2478 GPa. The value of BREF corresponds to a sound speed of 1.591 km/s.
- No changes were made to the 301 table.

COMMENTS.

- This EOS has a tension region for temperatures less than 800K for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- Pressure, energy and free energy are tabulated in the 301 table.

EOS NUMBER 7281

MATERIAL. Salt (Z=14, A=29.2214)

SOURCE. A. Merts and N. Magee

DATE. Nov 81 (orig data); Aug 92 (modifications)

REFS. LA-5068

COMPOSITION. NaCl

CODES. EOS - A Thomas-Fermi code for electron contribution with Barnes cold curve corrections.

RANGE. 25 densities, 0.0, 2.16e-6, ..., 2.16e4 g/cc,  
23 temperatures, 0.0, 116.1, 232.1, ..., 5.8e8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.26335 GPa, TREF=298.15K, RREF=2.165 g/cc and BREF=27.6222 GPa. The value of BREF corresponds to a sound speed of 3.5801 km/s. T=0.0 and 298.15 isotherms were added to the 301 table.

COMMENTS.

- This EOS does not consider known phase changes at moderately low pressure. A quick attempt to fill a request from Bob Deupree.
- This EOS is quite old so use with caution. It does not have any tension region and its treatment of the vaporization region is not realistic. The high value of PREF, necessitated by the treatment of the tension region, could cause problems in hydro calculations unless a two-state model is used to correct for it.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 7282

MATERIAL. Salt (Z=14, A=29.2214)

SOURCE. J. Johnson, S. Lyon

DATE. Jan 88 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. NaCl

CODES. GRIZZLY

RANGE. 73 densities, 0.0, 2.14e-6, ..., 4.27e4 g/cc,  
37 temperatures, 0.0, 145.1, 298.15, ..., 1.16e9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.1399 g/cc and BREF=22.585 GPa. The value of BREF corresponds to a sound speed of 3.3319 km/s.

- No changes were made to the 301 table.

## COMMENTS.

- Average atom modeling used throughout except for ideal gas portion of nuclear model where ideal mixing was used. TFD as calculated by candide in GRIZZLY was used for the electronic contribution. Chartjd nuclear model with jd gamma (igrun = 7). gamref = 1.70, debkel = 300, tmelt = 1074. Dgamma = (-3.0,-3.0) was adjusted to fit shock data at shock density of 0.868. Cold curve from shock data at shock density of 2.137. Us-up composed of four straight lines (up,us) = (0.0,3.35), (1.71,5.66), (2.53,6.30), (3.18,7.64), (5.0,10.1). Cmat = 1.98, ecohkc = 76.7, fac1j = 0.115. 301 table has van der Waals loops. Critical temperature is 3440 K.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7283

MATERIAL. Salt (Z=14, A=29.2214)

SOURCE. J. Johnson, S. Lyon

DATE. Jan 88 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. NaCl(CaSO4)0.0477

CODES. GRIZZLY

RANGE. 73 densities, 0.0,2.24e-6,...,4.48e4 g/cc,  
37 temperatures, 0.0,145.1,298.15,...,1.16e9 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.2431 g/cc and BREF=23.6693 GPa. The value of BREF corresponds to a sound speed of 3.3335 km/s.
- No changes were made to the 301 table.

## COMMENTS.

- This is the same as 7282 except for the following differences: zbar = 13.666, abar = 28.404, rhoref = 2.24, tmelt = 1070, ecohkc = 78, tcrit = 3500 k.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7330

MATERIAL. Calcium Carbonate (Z=10.0, A=20.0179)

SOURCE. F. H. Ree (LLNL, H-Division)

DATE. Jun 83 (orig data); Aug 92 (modifications)

REFS. F. H. Ree, "Equations of State of CaCO3 and its Mixtures with H2O", Lawrence Livermore National Laboratory Report UCRL-53113 (1981).

COMPOSITION. CaCO3

CODES. Gray, Tiger, Cheq, Occipital, Tfnuc

RANGE. 93 densities, 0.0,1.0e-6,...,1000 g/cc,  
42 temperatures, 0.0,290.11,348.1,...,2.9e8 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give PREF=1.013e-4 GPa, TREF=290.11K (STP conditions), RREF=2.71 g/cc and BREF=73.6 GPa. The value of

BREF was chosen to give about the right sound speed, 5.211 km/s.

- A  $\rho=0.0$  isochore and  $T=0.0$  isotherm were added to the 301 table.

COMMENTS.

- This is a wide-range multiphase equation of state which covers a density range between  $1.0 \times 10^{-6}$  and  $1.0 \times 10^3$  g per  $\text{cm}^3$  and a temperature range between 0.025 and  $2.5 \times 10^4$  ev. The physical models which were used to calculate the eos are as follows: (1) gray - a semi-empirical model which calculates an eos from the Gruneisen model for a solid, assuming that the solid is harmonic. It calculates the liquid state by modifying the solid free energy by an entropy correction associated with loss of order. Gray covers densities between 2.71 and 8.0 g per  $\text{cm}^3$  and temperatures from 0.025 to 1.0 ev. The solid was assumed to be in the aragonite phase. (2) Tiger-Cheq - these models were used in the low-temperature, low density region which is sensitive to the chemical equilibrium of  $\text{CaCO}_3$  and the dissociated species of  $\text{CaCO}_3$ . Tiger calculates the gaseous eos properties of the mixture using a bkw eos model. In the vapor-solid region, the code Cheq was used to solve the equilibrium compositions of chemical species by extent-of-reaction variable method. (3) Occipital - covers high-temperature, low density region.  $\text{CaCO}_3$  is assumed to be completely dissociated into electrons, ions, and neutral atoms. The concentrations of each are obtained from the Saha equation, and the thermodynamic properties are computed assuming that the mixtures behave like an ideal gas. (4) Tfnuc - calculates electronic contributions to the eos using Thomas-Fermi theory with Kirzhnits corrections for the wave nature of electrons and the electron exchange contribution. Nuclear contributions are calculated with a Gruneisen model at low temperature and the one-component plasma model at high temperature.
- This EOS has Maxwell constructions with no tension region. As a result, vaporization is treated correctly but the EOS will not give correct results in cases where spall should occur. Also, interpolation on the tables does not give the correct sound speed at the reference state.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 7331

MATERIAL. Calcite ( $Z=10.0$ ,  $A=20.018$ )

SOURCE. J. Barnes, S. Lyon

DATE. Jan 88 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION.  $\text{CaCO}_3$

CODES. GRIZZLY

RANGE. 72 densities,  $0.0, 2.71 \times 10^{-6}, \dots, 5.42 \times 10^4$  g/cc,

37 temperatures,  $0.0, 145.1, 298.15, \dots, 1.16 \times 10^9$  Kelvin.

MODIFICATIONS.

- The 201 table was modified to give  $P_{\text{REF}}=0.0$  GPa,  $T_{\text{REF}}=298.152$  K (STP conditions),  $R_{\text{REF}}=2.7116$  g/cc and  $B_{\text{REF}}=70.4604$  GPa. The value of  $B_{\text{REF}}$  corresponds to a sound speed of 5.1245 km/s.
- No changes were made to the 301 table.

COMMENTS.

- Average atom modeling used throughout except for ideal gas portion of nuclear model where ideal mixing was used. Tfd as calculated by candid in Grizzly was used for the electronic

contribution. Chartjd nuclear model with chartd gamma (igrun = 1). Gamref = 1.12, debkel = 750, tmelt = 1612. Cold curve from shock data. Us-up composed of three straight lines (up,us) = (0.0,5.13), (0.86,6.30), (1.74,6.30), (3.71,9.00). cmat=1.70, ecohkc=135.6, fac1j = 0.325. 301 table has van der Waals loops. Critical temperature is 10,250 K.

- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7380

MATERIAL. Quartz (Z=10, A=20.028)

SOURCE. J. Barnes, J. Rood

DATE. Aug 73 (orig data); Feb 92 (modifications)

REFS. None

COMPOSITION. SiO<sub>2</sub>

CODES. Sesame I

RANGE. 101 densities, 0.0,.0172,...,44080 g/cc,

23 temperatures, 0.0,290.12,580.2,...,3.71E8 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=290.121 K (STP conditions), RREF=2.1554 g/cc and BREF=33.8463 GPa. The value of BREF corresponds to a sound speed of 4.0905 km/s.
- In the tension region modifications were made to the 301 table at T<1160 K and density<1.765 g/cc to make pressure proportional to density and energy constant.

## COMMENTS.

- This EOS is quite old and should be used with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.121 even though it does not give the correct density.
- There is a tension region for temperatures below 1160 K.
- This EOS is not thermodynamically consistent in the vapor-liquid region. Maxwell constructions were put into the pressure table but not in the energy table.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

## EOS NUMBER 7381

MATERIAL. Quartz (Z=10, A=20.028)

SOURCE. R. Albers

DATE. Feb 81 (orig data); Jul 92 (modifications)

REFS. None

COMPOSITION. SiO<sub>2</sub>

CODES. EOSLTS, SUBT

RANGE. 36 densities, 0.0,2.2E-4,...,22040 g/cc,

54 temperatures, 0.0,293.16,580.2,...,1.16E9 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=293.16 K (STP conditions), RREF=2.2039 g/cc and BREF=31.7544 GPa. The value of BREF corresponds to a sound speed of 3.87 km/s.
- No changes were made to the 301 table.

## COMMENTS.

## Sandia EOS Data Base

- This EOS is quite old so use with caution.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than ~7750K.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

### EOS NUMBER 7383

MATERIAL. Polycrystal Quartz (Z=10, A=20.0281)

SOURCE. J. Johnson, S. Lyon

DATE. Nov 84 (orig data); Jul 92 (modifications)

REFS. None

COMPOSITION. SiO<sub>2</sub>

CODES. GRIZZLY

RANGE. 73 densities, 0.0, 2.65E-6, ..., 53000 g/cc,

37 temperatures, 0.0, 145.1, 298.15, ..., 1.16E9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.6498 g/cc and BREF=36.6777 GPa. The value of BREF corresponds to a sound speed of 3.7327 km/s.
- No changes were made to the 301 table.

#### COMMENTS.

- Average atom modeling throughout. TFD as calculated by Candide in GRIZZLY was used for the electronic contribution. Cold curve from shock data and sound velocities. Used Us-up composed of 3 straight lines, up = 0.0, 1.0, 2.41, 4.0, 26.76 and us = 3.75, 5.7, 5.7, 8.641, 38.87 respectively. Data from Chung and Simmons; Wackerle, Ragan, and McQueen; Fritz, and Hopson. Tfd matches made at a compression of 1.868. ecoh = 146 kcal per mole from B. Albers chartd nuclear model. Special gamma (igrun = 7) with gameps = 0.5, gamref = 0.653, dgamma1 = 1.1227, and dgamma2 = 0.0. This gamma fits data due to Wackerle and McQueen, Fritz, and Marsh. Debyeref = 950 kelvin from Lord and Morrow. This eos is pretty good for polycrystal quartz and only slightly less accurate for crystal quartz.
- This EOS is quite old so use with caution.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than ~7000K.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 7385

MATERIAL. Polycrystal Quartz (Z=10, A=20.028)

SOURCE. J. Barnes, S. Lyon

DATE. Jun 87 (orig data); Jul 92 (modifications)

REFS. None

COMPOSITION. SiO<sub>2</sub>

CODES. GRIZZLY

RANGE. 73 densities, 0.0, 2.65E-6, ..., 53000 g/cc,

37 temperatures, 0.0, 145.1, 298.15, ..., 1.16E9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.6499 g/cc and BREF=36.6961 GPa. The value of BREF corresponds to a sound speed of 3.7332 km/s.
- No changes were made to the 301 table.

## COMMENTS.

- This is the same as 7383 except the Chartjd nuclear model was used.
- This EOS is quite old so use with caution. One deficiency is
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than ~10000K.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7386

MATERIAL. Fused Quartz (Z=10, A=20.0281)

SOURCE. J. Boettger

DATE. Nov 88 (orig data); Jul 92 (modifications)

REFS. LA-11488-MS

COMPOSITION. SiO<sub>2</sub>

CODES. GRIZZLY

RANGE. 75 densities, 0.0, 2.2E-6, ..., 44080 g/cc,

39 temperatures, 0.0, 145.1, 298.15, ..., 1.16E9 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.204 g/cc and BREF=37.5313 GPa. The value of BREF corresponds to a sound speed of 4.1371 km/s.
- No changes were made to the 301 table.

## COMMENTS.

- The electronic contribution and the cold curve for high compressions were constructed by first applying tfd theory to each component separately and then using additive volume mixing. For compressions less than 2.1 the cold curve was derived from a 4 line fit to experimental hugoniot data defined by five (up,us) points- (0.00,4.09), (0.85,5.1), (2.25,5.1), (2.877,5.71), (4.494,8.461). The expanded cold curve uses a Lennard-Jones form with fac1j = 3.0 and ecohkc = 146. The chartjd nuclear model was used with debkel = 950, gamref = 0.65, tmelt = 1900. This eos is superior to 7381 for fused quartz. It is not intended as an eos for crystalline or polycrystalline quartz.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than ~6000K.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7390

MATERIAL. Westerly Granite (Z=10.272, A=20.669)

SOURCE. J. Barnes, J. Rood

DATE. Mar75, Jan 79 (orig data); Jul 92 (modifications)

REFS. None

COMPOSITION. SiO<sub>2</sub>[73.9%] Al<sub>2</sub>O<sub>3</sub>[14.9%] K<sub>2</sub>O[4.5%] CaO[3.3%] FeO[2.0%]  
(plus trace amounts of other oxides) by weight

## Sandia EOS Data Base

CODES. SESAME I

RANGE. 101 densities, 0.0,0.0205,...,5.254E+4 g/cc,

23 temperatures, 0.0,290.12,580.24,...,3.71E+8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=1.013E-4 GPa, TREF=290.12 K (STP conditions), RREF=2.5505 g/cc and a sound speed of 1.9698 km/s. A rho=0 isochore was added to the 301 table.

COMMENTS.

- This EOS is quite old so use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- This EOS does not have a tension region. It does not give the correct sound speed at the reference state.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 7410

MATERIAL. Alumina (Z=10, A=20.392)

SOURCE. J. Barnes, J. Rood

DATE. Nov 72, Jan 79 (orig data); Jul 92 (modifications)

REFS. None

COMPOSITION. Al2O3

CODES. SESAME

RANGE. 101 densities, 0.0,3.102E-2,...,3970 g/cc,

23 temperatures, 0.0,290.121,580.24,...,3.7E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=290.121 K, RREF=3.96114 g/cc and BREF=236.802 GPa. The value of BREF corresponds to a sound speed of 7.7584 km/s.
- A rho=0.0 isochore was added to the 301 table.

COMMENTS.

- This EOS is quite old so use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm.
- This EOS has van der Waals loops. Hence it gives a tension region for for temperatures less than ~2900K to use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- It appears Maxwell constructions were applied to temperatures above 2900K. A cross over of isochores occur at approximately 3.39 g/cc for temperatures greater than 2900K.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 7411

MATERIAL. Alumina (Z=10, A=20.392)

SOURCE. J. Barnes, S. Lyon

DATE. Jun 87 (orig data); Jul 92 (modifications)

REFS. LA-11058-MS

COMPOSITION. Al2O3

CODES. GRIZZLY

RANGE. 68 densities, 0.0,37,...,79400 g/cc,

37 temperatures, 0.0,145.06,298.152,...,1.16E9 Kelvin.

MODIFICATIONS.



- The 201 table was modified to give PREF=0.0 GPa, TREF=298.15 K (STP conditions), RREF=3.9704 g/cc and BREF=241.119 GPa. The value of BREF corresponds to a sound speed of 7.8197 km/s.
- No changes were made to the 301 table.

## COMMENTS.

- Average atom modeling throughout except for ideal gas portion of nuclear model where ideal mixing was used.
- TFD as calculated by candide in GRIZZLY was used for the electronic contribution. Chartjd nuclear model with chartd Gamma (igrun=1). Gamref=1.595 debkel=1034, tmelt=0,. Cold curve from shock data and sound speed. Used Us-up composed of a single straight line with (Up,us)=(0.0,7.93). CMAT=1.35, ecohkc=145, fac1j=0.5. 301 table has Van der Waals loops. Critical temperature is 14500K.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than ~12500K.
- A negative internal energy exists for temperatures less than TREF.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7440

MATERIAL. Hematite (Z=15.2, A=31.938)

SOURCE. J. Barnes, S. Lyon

DATE. Jun 87 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. Fe2O3

CODES. GRIZZLY

RANGE. 71 densities, 0.0,5e-6,...,1.0e5 g/cc,

37 temperatures, 0.0,145.06,298.152,...,1.16e9 Kelvin.

## MODIFICATIONS.

- The 201 table was modified to give PREF=0 GPa, TREF=298.152 K (STP conditions), RREF=5.0079 g/cc and BREF=191.385 GPa. The value of BREF corresponds to a sound speed of 6.215 km/s.
- No changes were made to the 301 table.

## COMMENTS.

- Average atom modeling used throughout except for ideal gas portion of nuclear model where ideal mixing was used. Tfd as calculated by candide in grizzly was used for the electronic contribution. Chartjd nuclear model with chartd gamma (igrun = 1). Gamref = 1.64, debkel = 610, tmelt = 1838. Cold curve from shock data and sound speed. Us-up composed of three straight lines (up,us) = (0.0,6.243), (0.95,7.50), (2.25,7.50), (3.20,8.75). Cmat = 1.58, ecohkc = 114.2, fac1j = 0.5. 301 table has Van Der Waals loops. Critical temperature is 12,000 k.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7450

MATERIAL. Calcium Oxide (Z=14, A=28.04)

SOURCE. J. Barnes, S. Lyon

DATE. Jun 87 (orig data); Aug 92 (modifications)

REFS. None

## Sandia EOS Data Base

COMPOSITION. CaO

CODES. GRIZZLY

RANGE. 72 densities, 0.0, 2.98e-6, ..., 5.96e4 g/cc,  
37 temperatures, 0.0, 145.06, 298.152, ..., 1.16e9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.9824 g/cc and BREF=37.7778 GPa. The value of BREF corresponds to a sound speed of 3.6963 km/s.
- No changes were made to the 301 table.

COMMENTS.

- Average atom modeling used throughout except for ideal gas portion of nuclear model where ideal mixing was used. Tfd as calculated by candide in grizzly was used for the electronic contribution. Chartjd nuclear model with chartd gamma (igrun = 1). Gamref = 2.40, debkel = 640, tmelt = 2853. Cold curve from shock data. Us-up composed of three straight lines (up,us) = (0.0, 3.70), (2.30, 7.70), (3.05, 7.70), (3.55, 8.55). Cmat = 1.72, ecohkc = 126.7, fac1j = 0.25. 301 table has van der Waals loops. Critical temperature is 9000 K.
- This EOS is quite old so use with caution.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 7460

MATERIAL. Periclase (Z=10, A=20.156)

SOURCE. J. Barnes, S. Lyon

DATE. Jan 88 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. MgO

CODES. GRIZZLY

RANGE. 73 densities, 0., 0.0, 3.58e-6, ..., 7.17e4 g/cc,  
37 temperatures, 0., 0.0, 145.06, 298.152, ..., 1.16e9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=3.5847 g/cc and BREF=160.388 GPa. The value of BREF corresponds to a sound speed of 6.7292 km/s.
- No changes were made to the 301 table.

COMMENTS.

- Average atom modeling used throughout except for ideal gas portion of nuclear model where ideal mixing was used. Tfd as calculated by candide in grizzly was used for the electronic contribution. Chartjd nuclear model with chartd gamma (igrun = 1). Gamref = 1.72, debkel = 938, tmelt = 3125. Cold curve from shock data. Us-up composed of one straight line with c0 = 6.78 and s = 1.292. Cmat = 1.98, ecohkc = 118, fac1j = 0.26. 301 table has van der Waals loops. Critical temperature is 7850 K.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 7510

MATERIAL. Dolomite (Z=9.2, A=18.44)

SOURCE. J. Johnson, S. Lyon

DATE. Jan 88 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. CaMg(CO<sub>3</sub>)<sub>2</sub>

CODES. GRIZZLY

RANGE. 69 densities, 0.0, 2.82e-6, ..., 5.64e4 g/cc,  
37 temperatures, 0.0, 145.06, 298.152, ..., 1.16e9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.8229 g/cc and BREF=80.8488 GPa. The value of BREF corresponds to a sound speed of 5.3815 km/s.
- No changes were made to the 301 table.

COMMENTS.

- Average atom modeling used throughout except for ideal gas portion of nuclear model where ideal mixing was used. Tfd as calculated by candide in grizzly was used for the electronic contribution. Chartjd nuclear model with chartd gamma (igrun = 1). Gamref = 1.2, debkel = 750, tmelt = 1300. Cold curve from shock data. Us-up composed of one straight line with c0=5.4 and s=1.15. cmat = 1.70, ecoh = 0.3, fac1j = 0.25. 301 table has van der Waals loops. Critical temperature is 8525 K.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- Pressure, energy and free energy are tabulated in the 301 table.

#### EOS NUMBER 7520

MATERIAL. Mica (Z=6.8697, A=13.524)

SOURCE. J. Barnes, J. Rood

DATE. May 74 Jan 79 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. O[56.1%] Si[16.7%] Mg[12.6%] Al[7.6%] Fe[4.5%]  
H[2.4%] Weight percent

CODES. SESAME I

RANGE. 101 densities, 0.0, 2.11e-2, ..., 5.4e4 g/cc,  
23 temperatures, 0.0, 290.12, 580.2, ..., 3.71e8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=1.013e-4 GPa, TREF=290.12 K (STP conditions), RREF=2.6214 g/cc and BREF=12.5654 GPa. The value of BREF corresponds to a sound speed of 2.1925 km/s. A rho=0.0 isochore was added to the 301 table.

COMMENTS.

- This EOS is quite old so use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- This EOS has Maxwell constructions with no tension region.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

#### EOS NUMBER 7530

MATERIAL. Basalt (Z=10.665, A=22.574)

SOURCE. J. Barnes, S. Lyon

DATE. Jan 88 (orig data); Jun 92 (modifications)

REFS. Lams report in progress

COMPOSITION. O[60.11%] Si[18.26%] Al[5.96%] Ca[4.01%]  
Fe[3.48%] Mg[3.39%] H[2.18%] Na[1.56%] Ti[0.55%] K[0.38%]

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P[0.07%] Mn[0.06%] by number  
CODES. GRIZZLY  
RANGE. 71 densities, 0.0,2.87E-6,...,5.74E+4 g/cc,  
37 temperatures, 0.0,145.06,298.152,...,1.16E+9 Kelvin.  
MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=2.86594 g/cc and BREF=75.8994 GPa. The value of BREF corresponds to a sound speed of 5.1704 km/s.
- No changes were made to the 301 table.

### COMMENTS.

- Average atom modeling used throughout except for ideal gas portion of nuclear model where ideal mixing was used.
- TFD as calculated by candide in GRIZZLY was used for the electronic contribution. Chartjd nuclear model with chartd Gamma (igrun=1). Gamref= 1.17, debkel = 851, tmelt = 2158. Cold curve from shock data. Us-up composed of three straight lines (up,us) = (0.0,5.21), (0.54,5.98), (1.75,5.98), (4.00,9.25). CMAT= 1.76, ecohkc = 137, faclj = 0.185. The reference gamma, debye temperature and cohesive energy for the mixture were taken to be the weighted sum of the corresponding parameter values for each of the major molecular components. 301 table has Van der Waals loops. Critical temperature is 6675 K.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than ~5300K.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7541

MATERIAL. Carbon Phenolic (Z=4.648, A=9.0105)  
SOURCE. J. D. Johnson  
DATE. Apr 81 (orig data); Mar 92 (modifications)  
REFS. 111 Shock Compendium, WX-3 Memo (9-20-79), private communication with F. Mortonson (X-2)  
COMPOSITION. C[64.18%] H[29.5%] O[5.98%] N[0.34%] by moles  
CODES. EOSLTS, CANDIDE  
RANGE. 56 densities, 0.,1.52E-3,3.03E-3,...,1.52E3 g/cc,  
25 temperatures, 0.,298.12,485.67,835.44,...,3.71E8 Kelvin.

### MODIFICATIONS.

- The 201 table was modified to give RREF=1.45025, TREF=298.12, and BREF=13.246 GPa. The value of BREF corresponds to a sound speed of 3.0515 km/s.
- No changes were made to the 301 table.

### COMMENTS.

- This EOS does not have Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than 6350K.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

## EOS NUMBER 7542

MATERIAL. Carbon Phenolic (Z=4.75910, A=9.25862)  
SOURCE. J. Johnson, S. Lyon

DATE. Feb 87 (orig data); Mar 92 (modifications)

REFS. None

COMPOSITION. C[66%] H[26.93%] O[3.49%] N[3.58%] by moles

CODES. GRIZZLY

RANGE. 68 densities, 0., 1.5E-6, 3.0E-6, ..., 3.0E4 g/cc,

37 temperatures, 0., 145.06, 298.15, 580.24, ..., 1.16E9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give RREF=1.49945, TREF=298.152, and BREF=14.7186 GPa. The value of BREF corresponds to a sound speed of 3.1499 km/s.
- No changes were made to the 301 table.

COMMENTS.

- Electronic table is mix of thermal TFD for 4 elements. Nuclear table is from first version of CHARTFD (before Debye-Huckel). Cold curve comes from shock data procedure. Us-up input is up = 0, 3.0 with us=3.15, 6.15. ECOH=150 kcal per average atom mole, GAMREF=0.5, and DEBREF=1000 K. We used IGRUN=7 with GAMEPS=0.5, 1.0 and DGAMMA= 0., 0.. The TFD match compression is 2.0. The default TMELT is used. The Hugoniot is compared to data in the compendia while all other input numbers are intelligent guesses.
- This EOS does not have Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly. It does give the correct sound speed at the reference state.
- There is a tension region for temperatures less than 7600K.
- A negative internal energy exists for temperatures less than TREF.
- Pressure, energy and free energy are tabulated in the 301 table.

EOS NUMBER 7560

MATERIAL. Polyurethane (Z=3.76290, A=7.03840)

SOURCE. J. Barnes, S. Lyon

DATE. Oct 74 Jan 79 (orig data); Mar 92 (modifications)

REFS. None

COMPOSITION. C[62.3%] O[23.3%] N[7.3%] H[7.1%] by weight

CODES. SESAME I

RANGE. 101 densities, 0., 9.9E-3, 1.9E-2, ..., 2.53E4 g/cc,

23 temperatures, 0., 290.121, 580.24, 1160.5, ..., 3.71E8 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=1.013E-4 GPa, TREF=290.12K (STP conditions), RREF=1.01305 g/cc and BREF=4.35 GPa. BREF corresponds to a sound speed of 2.073 km/s.
- No changes were made to the 301 table.

COMMENTS.

- This EOS is quite old so use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- Behavior in the vapor-liquid region appears anomalous and is probably not trustworthy.
- Another problem with this EOS is that it does not have a tension region, so it will not predict fracture in dynamic calculations.
- The interpolation scheme does not give correct sound speed at ambient temperature and density. The value in the 201 table was taken from experiment, so that some of the problems could be corrected using the two-state model.

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- No zero pressure values exist in the 301 table.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

### EOS NUMBER 7561

MATERIAL. Polyurethane (Z=3.645, A=6.782)

SOURCE. J. Barnes, S. Lyon

DATE. Dec 88 (orig data); Mar 92 (modifications)

REFS. None

COMPOSITION. C[11]H[16]N[1]O[3]

CODES. GRIZZLY

RANGE. 73 densities, 0., 1.26E-6, 2.53E-6, ..., 2.53E4 g/cc,  
38 temperatures, 0., 145.06, 298.15, 580.24, ..., 1.16E9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give PREF=1.013E-4, RREF=1.26405, TREF=298.152, and BREF=5.40 GPa. BREF corresponds to a sound speed of 2.073 km/s.
- No changes were made to the 301 table.

#### COMMENTS.

- Average atom modeling throughout except for ideal gas portion of nuclear model where ideal mixing was used. TFD as calculated by candide in GRIZZLY was used for the electronic contribution. CHARTJD nuclear model with CHARTD GAMMA (IGRUN=1). GAMREF=1.10, DEBKEL=167, TMELT=450. Cold curve from shock data and sound velocity. (up,us) points are (0.0,2.068), (0.6,3.50), (2.69,6.78), (3.58,7.44), (5.13,9.75). In order to match the critical point data, we set ECOHFC=17 and FACLJ=0.15. In order to get a total pressure of 1 bar at room temperature and normal density, we rescaled the cold curve using RHO0=1.31765. TFD match compression was 2.11.
- A problem with this EOS is that it does not have a tension region, so it will not predict fracture in dynamic calculations.
- The interpolation scheme does not give correct sound speed at ambient temperature and density. The value in the 201 table was taken from experiment, so that some of the problems could be corrected using the two-state model.
- A negative internal energy exists for temperatures less than TREF.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 7590

MATERIAL. Polystyrene (Z=3.5, A=6.51)

SOURCE. J. Barnes, A. Lindstrom

DATE. Jan76 (orig data); Jul 92 (modifications)

REFS. T-4 Notebook

COMPOSITION. CH

CODES. SESAME I, MAPLE, MAXWELL

RANGE. 101 densities, 0.0, 8.156E-3, ..., 20880 g/cc,  
23 temperatures, 0.0, 290.121, 580.2, ..., 3.71E+8 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give PREF=1.013E-4 GPa, TREF=290.121 K (STP conditions), RREF=0.76225 g/cc and BREF=0.2331 GPa. The value of BREF corresponds to a sound speed of 0.55376 km/s.
- No changes were made to the 301 table.

#### COMMENTS.

- The existing 7590 table has been updated using fixtab3. The

only change involved fixing 5 energy points by a few percent to prevent crossing isotherms and negative specific heats. The range fixed was at densities between 5.22e3 and 2.088e4 (the 3 highest densities) and temperatures between 2.32e6 and 5.80e6. For further information, contact Bob Albers (t-4).

- This EOS is quite old so use with caution. One deficiency is that room temperature density had been used for the zero-K isotherm. The reference temperature was chosen to be 290.12 even though it does not give the correct density.
- This EOS has Maxwell constructions but no tension region. It does not give the correct sound speed at the reference state.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

#### EOS NUMBER 7591

MATERIAL. Polystyrene (Z=3.5, A=6.51)

SOURCE. J. Barnes, S. Lyon

DATE. Aug 86 (orig data); Jul 92 (modifications)

REFS. LAMS Report

COMPOSITION. CH

CODES. GRIZZLY

RANGE. 70 densities, 0.0, 1.04E-6, ..., 20880 g/cc,  
41 temperatures, 0.0, 298, 580.2, ..., 1.16E+9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298 K (STP conditions), RREF=0.9918 g/cc and BREF=0.0945 GPa. The value of BREF corresponds to a sound speed of 0.3166 km/s.
- No changes were made to the 301 table.

#### COMMENTS.

- Average atom modeling throughout except for ideal gas portion of nuclear model where ideal mixing was used.
- TFD as calculated by candide in GRIZZLY was used for the electronic contribution. Chartjd nuclear model with chartd gamma (igrun=1). Gamref adjusted to 0.5 to reproduce shock data for foamed polystyrene at initial density of 0.3. Debkel=258, tmelt=600. Cold curve from shock data and sound velocity. Used us-up composed of 3 straight lines with up = 0.0, 3.25, 4.0, 7.15 and us = 2.0, 7.5, 7.5, 12.0 respectively. Data from lasl shock compendium. Tfd match made at compression of 2.47. ecoh=112 calculated from heat of vaporization of carbon and dissociation energy of hydrogen. Fac1j=1.0. 301 table has Maxwell constructions
- No tension region exists.
- Pressure, energy and free energy are tabulated in the 301 table.

#### EOS NUMBER 7592

MATERIAL. Polystyrene (Z=3.5, A=6.51)

SOURCE. J. Barnes, S. Lyon

DATE. Nov 88 (orig data); Jul 92 (modifications)

REFS. None

COMPOSITION. CH

CODES. GRIZZLY

RANGE. 73 densities, 0.0, 1.04E-6, ..., 20880 g/cc,  
41 temperatures, 0.0, 145.06, 298, ..., 1.16E+9 Kelvin.

#### MODIFICATIONS.

- The 201 table was modified to give PREF=1.013E-4 GPa,

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TREF=298.152 K (STP conditions), RREF=1.044 g/cc and  
BREF=1.7407 GPa. The value of BREF corresponds to  
a sound speed of 1.3016 km/s.

- No changes were made to the 301 table.

### COMMENTS.

- Average atom modeling throughout except for ideal gas portion of nuclear model where ideal mixing was used.
- TFD as calculated by candide in GRIZZLY was used for the electronic contribution. Chartjd nuclear model with chartd gamma (igrun=1). gamref = 0.565, debkel = 222, tmelt = 510. Cold curve from shock data and sound velocity. (us,up) data points (0.0,1.898), (0.77,3.47), (2.30,6.29), (3.80,7.35), (5.35,9.57). In order to match critical point data, we set ecohkc = 15 and fac1j = 0.20. In order to get a total pressure of 1 bar at room temperature and normal density, we rescaled the cold curve with rho0 = 1.071. Tfd match compression was 2.268. 301 table has Maxwell constructions.
- No tension region exists.
- It does not give the correct sound speed at the reference state.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 7601

MATERIAL. Epoxy (Z=3.2407, A=5.9134)

SOURCE. J. Johnson

DATE. July 84 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. C[0.347] O[0.048] H[0.577] N[0.028] by number  
fraction

CODES. GRIZZLY

RANGE. 69 densities, 0.0,1.18e-6,...,2.37e4 g/cc,

37 temperatures, 0.0,145.06,298.152,...,1.16e9 Kelvin.

### MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=1.1853 g/cc and BREF=8.0295 GPa. The value of BREF corresponds to a sound speed of 2.7356 km/s.
- No changes were made to the 301 table.

### COMMENTS.

- Average atom modeling throughout. Tfd as calculated by candide in grizzly was used for electronic contribution. Cold curve obtained from shock data in lasl compendium. Tfd match shifted to compression of 1.9 and ecoh = 57 mj per kg. Chartd nuclear and gammodels with gamma0 = 0.8. Theta0 found from poisson = 0.333.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than 3000K.
- Pressure, energy and free energy are tabulated in the 301 table.

### EOS NUMBER 7602

MATERIAL. Epoxy (Z=3.2407, A=5.9134)

SOURCE. J. Johnson

DATE. Nov 84 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. C[0.347] O[0.048] H[0.577] N[0.028] by number  
fraction



CODES. EOSCRAY, CANDIDE

RANGE. 66 densities, 0., 0.0, 1.32e-6, ..., 1323 g/cc,

27 temperatures, 0., 0.0, 145.06, 298.129, ..., 1.16e9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=1.013e-4 GPa, TREF=298.129 K (STP conditions), RREF=1.185 g/cc and BREF=4.011 GPa. The value of BREF corresponds to a sound speed of 1.9019 km/s.
- No changes were made to the 301 table.

COMMENTS.

- This eos is the same modeling as 7601 except maxwell constructions were made. Because we had to switch codes to do the maxwell constructions, small differences between the two eos's are to be expected. If two-temperature tables are needed for this material, the two-temperature tables from 7601 may be used.
- This EOS has Maxwell constructions with no tension region. Note that this results in an incorrect sound speed when interpolating from the tables.
- Only pressure and energy are tabulated in the 301 table. Entropy and free energy are not included.

EOS NUMBER 7610

MATERIAL. Beryllium Oxide (Z=6, A=12.506)

SOURCE. J. Barnes, S. Lyon

DATE. Mar86 (orig data); Aug 92 (modifications)

REFS. LAMS Report

COMPOSITION. BeO

CODES. GRIZZLY

RANGE. 68 densities, 0.0, 3.01e-6, ..., 60200 g/cc,

37 temperatures, 0.0, 145.06, 298.152, ..., 1.16e9 Kelvin.

MODIFICATIONS.

- The 201 table was modified to give PREF=0.0 GPa, TREF=298.152 K (STP conditions), RREF=3.01 g/cc and BREF=214.215 GPa. The value of BREF corresponds to a sound speed of 8.4591 km/s.
- No changes were made to the 301 table.

COMMENTS.

- Constructed with modified morse cold curve, cowan nuclear model and 3-coefficient virial match. Electronic thermal contribution was obtained from average-atom tfd calculations. Calculated shock hugoniot is in good agreement with experimental data above 400 kbar. Shock data at lower stresses shows effects of extremely high hugoniot elastic limit. Calculated vapor pressures are in fair agreement with limited experimental values available.
- This EOS has van der Waals loops and no Maxwell constructions. Hence it gives a tension region for use with fracture models but does not describe vaporization correctly.
- There is a tension region for temperatures less than ~9000K.
- Pressure, energy and free energy are tabulated in the 301 table.

EOS NUMBER 7750

MATERIAL. Lucite (Z=3.6, A=6.674)

SOURCE. J. Barnes, S. Lyon

DATE. Dec 88 (orig data); Aug 92 (modifications)

REFS. None

COMPOSITION. C5H8O2

CODES. GRIZZLY

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RANGE. 73 densities, 0.0,1.19e-6,...,2.37e4 g/cc,  
37 temperatures, 0.0,145.06,298.152,...,1.16e9 Kelvin.

### MODIFICATIONS.

- The 201 table was modified to give PREF=1.013e-4 GPa, TREF=298.152 K (STP conditions), RREF=1.186 g/cc and BREF=1.94084 GPa. The value of BREF corresponds to a sound speed of 1.298 km/s.
- No changes were made to the 301 table.

### COMMENTS.

- Average atom modeling throughout except for ideal gas portion of nuclear model where ideal mixing was used. Tfd as calculated by candide in grizzly was used for the electronic contribution. Chartjd nuclear model with chartd gamma (igrun=1). Gamref = 1.12, debkel = 222, tmelt = 443. cold curve from shock data and sound velocity. (up,us) data points (0.0,2.223), (0.50,3.40), (2.90,7.09), (3.24,7.33), (5.25,9.80). In order to match critical point data, we set ecokc = 15 and fac1j = 0.17. In order to get a total pressure of 1 bar at room temperature and normal density, we rescaled the cold curve with rho0 = 1.21705. Tfd match compression was 2.154. 301 table has maxwell constructions.
- There is no a tension region - sound speed from interpolation on table is probably not accurate.
- Pressure, energy and free energy are tabulated in the 301 table.

## EOS NUMBER 7931

MATERIAL. Sylgard 184 (silicone rubber) (z=4.2, a=7.84)

SOURCE. F. Dowell

DATE. May 85

REFS. LAMS report, to be published

COMPOSITION. wt% - C(30.9), H(7.4), Si(37.8), O(23.9).  
approximate formula - Si(CH3)2O.

CODES. GRIZZLY, FIXTB32

RANGE. 68 densities, 0.,1.E-6,1.E-5,...,2.1E+3 g/cc,  
33 temperatures, 0.,100.,200,298.15,...,1.2E9 Kelvin.

### MODIFICATIONS.

The 201 table was modified to give RREF=1.0373, TREF=298.15, and BREF=2.6270 GPa. The 301 table predicts a sound speed of 1.884. No changes were made to the 301 table.

### COMMENTS.

- This EOS does not have Maxwell constructions and so has a tension region for temperatures below 400 K. Between 400 and 900 K, the pressures are not monotonic below normal density, although the EOS does not actually go into tension.
- Pressure, energy, and free energy are tabulated in the 301 table.

## Distribution

### External Distribution

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